

## Bis[ $\mu$ -methylenebis(diphenylphosphine)]-bis[(5-nitro-1,10-phenanthroline)-silver(I)] bis(hexafluoridoantimonate)

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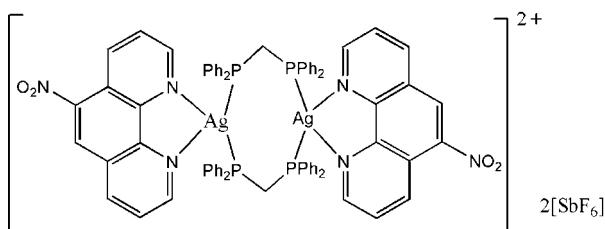
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Key indicators: single-crystal X-ray study;  $T = 293\text{ K}$ ; mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$ ; disorder in main residue;  $R$  factor = 0.030;  $wR$  factor = 0.060; data-to-parameter ratio = 10.1.

In the title compound,  $[\text{Ag}_2(\text{C}_{12}\text{H}_7\text{N}_3\text{O}_2)_2(\text{C}_{25}\text{H}_{22}\text{P}_2)_2](\text{SbF}_6)_2$ , the two  $\text{Ag}^{\text{I}}$  atoms are bridged by the two methylenebis(diphenylphosphine) ligands and an eight-membered centrosymmetric metallacyclic ring is formed. The metal atom exhibits a distorted tetrahedral coordination geometry, coordinated by two P atoms of the bridging ligands and two N atoms of the chelating 5-nitro-1,10-phenanthroline ligand. The latter ligand shows minor disorder, adopting two orientations with site occupancy factors of 0.84 and 0.16.

### Related literature

For related literature, see: Ho & Bau (1983); Smith & Cagle (1947).



### Experimental

#### Crystal data

$[\text{Ag}_2(\text{C}_{12}\text{H}_7\text{N}_3\text{O}_2)_2(\text{C}_{25}\text{H}_{22}\text{P}_2)_2](\text{SbF}_6)_2$	$\beta = 117.936(2)^\circ$
	$V = 3588.5(4)\text{ \AA}^3$
$M_r = 1906.38$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 12.8034(7)\text{ \AA}$	$\mu = 1.46\text{ mm}^{-1}$
$b = 23.3993(10)\text{ \AA}$	$T = 293(2)\text{ K}$
$c = 13.5580(11)\text{ \AA}$	$0.35 \times 0.35 \times 0.28\text{ mm}$

#### Data collection

Rigaku Mercury 70 CCD diffractometer	22441 measured reflections
Absorption correction: multi-scan ( <i>CrystalClear</i> ; Rigaku, 2000)	6301 independent reflections
$T_{\min} = 0.816$ , $T_{\max} = 1.000$	5851 reflections with $I > 2\sigma(I)$
(expected range = 0.543–0.665)	$R_{\text{int}} = 0.026$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	486 restraints
$wR(F^2) = 0.060$	H-atom parameters constrained
$S = 1.11$	$\Delta\rho_{\max} = 0.66\text{ e \AA}^{-3}$
6301 reflections	$\Delta\rho_{\min} = -0.70\text{ e \AA}^{-3}$
623 parameters	

**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ag—N1	2.392 (6)	Ag—P1	2.4491 (7)
Ag—P2	2.3982 (7)	Ag—N2	2.451 (5)
N1—Ag—P2	115.8 (3)	N1—Ag—N2	68.51 (15)
N1—Ag—P1	100.1 (3)	P2—Ag—N2	103.1 (2)
P2—Ag—P1	144.11 (3)	P1—Ag—N2	90.9 (2)

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2121).

### References

- Bruker (1999). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.  
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Rigaku (2000). *CrystalClear*. Version 1.3.6. Rigaku Corporation, Tokyo, Japan.  
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
Smith, G. F. & Cagle, F. W. M. (1947). *J. Org. Chem.* **12**, 781–784.

## **supplementary materials**

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## Bis[ $\mu$ -methylenebis(diphenylphosphine)]bis[(5-nitro-1,10-phenanthroline)silver(I)]bis(hexafluoridoantimonate)

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### Comment

The title compound,  $[\text{Ag}_2(\text{methylenebis}(\text{diphenylphosphine}))_2(5\text{-nitro-1,10-phenanthroline})_2](\text{SbF}_6)_2$ , is formed by self-assembly between the metal diphosphine compound  $[\text{Ag}_2(\text{methylenebis}(\text{diphenylphosphine}))_2](\text{SbF}_6)_2$  and 5-nitro-1,10-phenanthroline. In the crystal structure, the complex cation exists as a centrosymmetric dimer. Perspective view of the title compound is given in Fig. 1. The two methylenebis(diphenylphosphine) molecules bridge two  $\text{Ag}(5\text{-nitro-1,10-phenanthroline})$  moieties to form an eight-membered  $\text{Ag}_2\text{P}_4\text{C}_2$  metallacyclic ring with the 5-nitro-1,10-phenanthroline ligand chelating Ag atoms. The P1—Ag—P2 angle of  $144.11(3)^\circ$  is much larger than the N1—Ag—N2 angle of  $68.59(10)^\circ$ , indicating a distorted tetrahedral coordination geometry around the silver atom.

### Experimental

$[\text{Ag}_2(\text{methylenebis}(\text{diphenylphosphine}))_2](\text{SbF}_6)_2$  (Ho & Bau, 1983) and 5-nitro-1,10-phenanthroline (Smith & Cagle, 1947) were prepared according to the literature procedures. The title compound was prepared by reacting 0.25 mmol of  $[\text{Ag}_2(\text{bis}(\text{diphenylphosphino}))_2](\text{SbF}_6)_2$  with 0.5 mmol 5-nitro-1,10-phenanthroline in 15 ml  $\text{CH}_3\text{CN}$  at room temperature for 1 h. The resulting mixture was evaporated to dryness using Schlenk techniques. The solid product was recrystallized from a mixture of 15 ml  $\text{CH}_2\text{Cl}_2$  and 10 ml  $\text{CH}_3\text{OH}$  giving yellow crystals suitable for X-ray analysis.

### Refinement

All H atoms were included in calculated positions with C—H = 0.93 Å to 0.97 Å with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . Large anisotropic displacement parameters of the phenanthroline ligand and two high residual peaks in a difference map indicated a possible disorder of this ligand with the residual peaks attributed to a second position of the nitro group. The disorder of the 5-nitro-1,10-phenanthroline fragment was resolved into two partial-occupancy orientations and the occupancy factors were refined at 0.842 (4) and 0.158 (4). The atoms from the disordered unit were refined with the 'SIMU 0.01' restraint.

### Figures

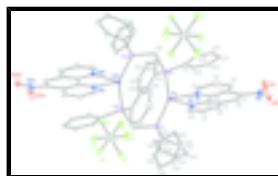


Fig. 1. *ORTEP* view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level and all hydrogen atoms were omitted for clarity. Atoms with the suffix A were generated by the symmetry operation  $-x, -y, 2 - z$ .

## supplementary materials

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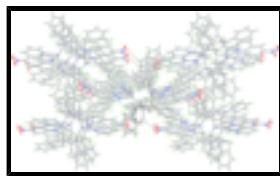


Fig. 2. Crystal packing of the title compound

### Bis[ $\mu$ -methylenebis(diphenylphosphine)]bis[(5-nitro-1,10-phenanthroline)silver(I)] bis(hexafluoridoantimonate)

#### Crystal data

$[\text{Ag}_2(\text{C}_{12}\text{H}_7\text{N}_3\text{O}_2)_2(\text{C}_{25}\text{H}_{22}\text{P}_2)_2](\text{SbF}_6)_2$	$F_{000} = 1880$
$M_r = 1906.38$	$D_x = 1.764 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 12.8034 (7) \text{ \AA}$	Cell parameters from 7865 reflections
$b = 23.3993 (10) \text{ \AA}$	$\theta = 3.0\text{--}25.0^\circ$
$c = 13.5580 (11) \text{ \AA}$	$\mu = 1.46 \text{ mm}^{-1}$
$\beta = 117.936 (2)^\circ$	$T = 293 (2) \text{ K}$
$V = 3588.5 (4) \text{ \AA}^3$	Prism, yellow
$Z = 2$	$0.35 \times 0.35 \times 0.28 \text{ mm}$

#### Data collection

Rigaku Mercury 70 CCD diffractometer	6301 independent reflections
Radiation source: fine-focus sealed tube	5851 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.026$
Detector resolution: 14.6306 pixels $\text{mm}^{-1}$	$\theta_{\text{max}} = 25.0^\circ$
$T = 293(2) \text{ K}$	$\theta_{\text{min}} = 3.0^\circ$
$\omega$ scans	$h = -15 \rightarrow 15$
Absorption correction: multi-scan (CrystalClear; Rigaku, 2000)	$k = -27 \rightarrow 26$
$T_{\text{min}} = 0.816$ , $T_{\text{max}} = 1.000$	$l = -16 \rightarrow 15$
22441 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
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.0186P)^2 + 5.1P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
6301 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
623 parameters	$\Delta\rho_{\text{max}} = 0.66 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.70 \text{ e \AA}^{-3}$

486 restraints  
 Primary atom site location: structure-invariant direct methods

### Special details

**Experimental.** 2007-03-05 # Formatted by publCIF

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^* / U_{\text{eq}}$	Occ. (<1)
Ag	0.023652 (17)	-0.075515 (9)	1.091671 (17)	0.01867 (6)	
P1	-0.17901 (6)	-0.06326 (3)	0.94206 (6)	0.01775 (16)	
P2	0.19380 (6)	-0.02588 (3)	1.22857 (6)	0.01697 (15)	
C21	-0.2634 (2)	-0.00996 (12)	0.9721 (2)	0.0216 (6)	
C22	-0.3864 (3)	-0.00586 (13)	0.9110 (3)	0.0247 (7)	
H22A	-0.4286	-0.0325	0.8555	0.030*	
C23	-0.4457 (3)	0.03785 (14)	0.9330 (3)	0.0326 (8)	
H23A	-0.5274	0.0409	0.8913	0.039*	
C24	-0.3838 (3)	0.07685 (15)	1.0167 (3)	0.0401 (9)	
H24A	-0.4241	0.1059	1.0315	0.048*	
C25	-0.2625 (3)	0.07299 (15)	1.0786 (3)	0.0385 (8)	
H25A	-0.2211	0.0992	1.1351	0.046*	
C26	-0.2027 (3)	0.02995 (13)	1.0562 (3)	0.0280 (7)	
H26A	-0.1209	0.0276	1.0977	0.034*	
C31	-0.2520 (2)	-0.13177 (12)	0.9320 (2)	0.0205 (6)	
C32	-0.2280 (2)	-0.17707 (13)	0.8787 (2)	0.0253 (7)	
H32A	-0.1866	-0.1703	0.8389	0.030*	
C33	-0.2651 (3)	-0.23201 (13)	0.8845 (3)	0.0313 (8)	
H33A	-0.2483	-0.2620	0.8491	0.038*	
C34	-0.3271 (3)	-0.24197 (14)	0.9432 (3)	0.0357 (8)	
H34A	-0.3513	-0.2789	0.9480	0.043*	
C35	-0.3532 (3)	-0.19762 (15)	0.9945 (3)	0.0351 (8)	
H35A	-0.3960	-0.2046	1.0329	0.042*	
C36	-0.3163 (2)	-0.14242 (14)	0.9894 (3)	0.0274 (7)	
H36A	-0.3343	-0.1126	1.0242	0.033*	
C41	0.1816 (2)	-0.02647 (12)	1.3574 (2)	0.0200 (6)	
C42	0.2094 (3)	-0.07752 (14)	1.4183 (3)	0.0275 (7)	
H42A	0.2376	-0.1085	1.3948	0.033*	
C43	0.1952 (3)	-0.08225 (15)	1.5130 (3)	0.0330 (8)	

## supplementary materials

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H43A	0.2131	-0.1165	1.5525	0.040*	
C44	0.1546 (3)	-0.03626 (16)	1.5490 (3)	0.0353 (8)	
H44A	0.1466	-0.0393	1.6135	0.042*	
C45	0.1261 (3)	0.01406 (15)	1.4896 (3)	0.0352 (8)	
H45A	0.0983	0.0449	1.5138	0.042*	
C46	0.1388 (3)	0.01893 (13)	1.3932 (3)	0.0261 (7)	
H46A	0.1185	0.0529	1.3528	0.031*	
C51	0.3399 (2)	-0.05683 (13)	1.2753 (2)	0.0206 (6)	
C52	0.3518 (3)	-0.10922 (13)	1.2338 (3)	0.0283 (7)	
H52A	0.2852	-0.1281	1.1808	0.034*	
C53	0.4631 (3)	-0.13370 (15)	1.2712 (3)	0.0389 (9)	
H53A	0.4709	-0.1688	1.2430	0.047*	
C54	0.5617 (3)	-0.10585 (16)	1.3500 (3)	0.0371 (8)	
H54A	0.6360	-0.1223	1.3751	0.044*	
C55	0.5510 (3)	-0.05397 (16)	1.3916 (3)	0.0349 (8)	
H55A	0.6182	-0.0352	1.4439	0.042*	
C56	0.4403 (2)	-0.02935 (14)	1.3558 (3)	0.0262 (7)	
H56A	0.4332	0.0054	1.3856	0.031*	
C61	-0.2118 (2)	-0.04967 (12)	0.7965 (2)	0.0206 (6)	
H61A	-0.1595	-0.0726	0.7791	0.025*	
H61B	-0.2924	-0.0613	0.7469	0.025*	
C1	0.0907 (6)	-0.1990 (2)	1.0194 (7)	0.0286 (12)	0.842 (4)
H1A	0.1206	-0.1748	0.9843	0.034*	0.842 (4)
C2	0.0947 (6)	-0.2583 (2)	1.0054 (5)	0.0438 (16)	0.842 (4)
H2A	0.1270	-0.2729	0.9619	0.053*	0.842 (4)
C3	0.0510 (5)	-0.2940 (2)	1.0557 (5)	0.0445 (16)	0.842 (4)
H3A	0.0541	-0.3332	1.0471	0.053*	0.842 (4)
C4	0.0010 (5)	-0.2723 (2)	1.1206 (4)	0.0338 (12)	0.842 (4)
C5	-0.0497 (5)	-0.3045 (2)	1.1798 (5)	0.0424 (17)	0.842 (4)
C6	-0.1018 (4)	-0.2802 (2)	1.2341 (4)	0.0427 (13)	0.842 (4)
H6A	-0.1364	-0.3033	1.2666	0.051*	0.842 (4)
C7	-0.1057 (5)	-0.2198 (2)	1.2435 (4)	0.0323 (12)	0.842 (4)
C8	-0.1592 (4)	-0.1931 (2)	1.3008 (4)	0.0411 (12)	0.842 (4)
H8A	-0.1969	-0.2146	1.3324	0.049*	0.842 (4)
C9	-0.1552 (5)	-0.1351 (2)	1.3094 (4)	0.0417 (12)	0.842 (4)
H9A	-0.1903	-0.1165	1.3468	0.050*	0.842 (4)
C10	-0.0977 (5)	-0.1041 (2)	1.2612 (5)	0.0326 (13)	0.842 (4)
H10A	-0.0943	-0.0646	1.2690	0.039*	0.842 (4)
C11	-0.0517 (5)	-0.18563 (19)	1.1947 (5)	0.0235 (10)	0.842 (4)
C12	0.0005 (7)	-0.2113 (2)	1.1323 (5)	0.0251 (11)	0.842 (4)
N1	0.0456 (9)	-0.1765 (2)	1.0812 (9)	0.0238 (10)	0.842 (4)
N2	-0.0478 (8)	-0.12770 (18)	1.2050 (7)	0.0233 (10)	0.842 (4)
N3	-0.0420 (4)	-0.36777 (18)	1.1863 (4)	0.0676 (16)	0.842 (4)
O1	-0.0046 (4)	-0.39241 (17)	1.1320 (6)	0.121 (3)	0.842 (4)
O2	-0.0729 (8)	-0.3919 (2)	1.2455 (8)	0.095 (3)	0.842 (4)
C1'	0.110 (4)	-0.1903 (13)	1.011 (4)	0.023 (3)	0.158 (4)
H1'A	0.1420	-0.1628	0.9842	0.027*	0.158 (4)
C2'	0.116 (3)	-0.2481 (13)	0.987 (3)	0.027 (4)	0.158 (4)
H2'A	0.1480	-0.2585	0.9405	0.032*	0.158 (4)

C3'	0.075 (3)	-0.2885 (12)	1.031 (3)	0.028 (4)	0.158 (4)
H3'A	0.0816	-0.3269	1.0173	0.034*	0.158 (4)
C4'	0.023 (3)	-0.2733 (11)	1.098 (3)	0.024 (3)	0.158 (4)
C5'	-0.026 (2)	-0.3121 (10)	1.149 (2)	0.026 (4)	0.158 (4)
H5'A	-0.0234	-0.3511	1.1372	0.031*	0.158 (4)
C6'	-0.074 (3)	-0.2941 (10)	1.210 (3)	0.032 (4)	0.158 (4)
C7'	-0.086 (3)	-0.2346 (9)	1.228 (3)	0.026 (3)	0.158 (4)
C8'	-0.129 (2)	-0.2136 (10)	1.299 (2)	0.031 (4)	0.158 (4)
H8'A	-0.1587	-0.2390	1.3318	0.037*	0.158 (4)
C9'	-0.127 (3)	-0.1569 (10)	1.320 (2)	0.031 (3)	0.158 (4)
H9'A	-0.1576	-0.1433	1.3656	0.038*	0.158 (4)
C10'	-0.079 (3)	-0.1187 (11)	1.271 (3)	0.031 (3)	0.158 (4)
H10B	-0.0756	-0.0798	1.2862	0.037*	0.158 (4)
C11'	-0.034 (3)	-0.1943 (10)	1.185 (3)	0.025 (3)	0.158 (4)
C12'	0.012 (4)	-0.2131 (11)	1.114 (3)	0.022 (3)	0.158 (4)
N1'	0.059 (6)	-0.1739 (13)	1.072 (5)	0.020 (3)	0.158 (4)
N2'	-0.038 (5)	-0.1379 (11)	1.204 (4)	0.023 (3)	0.158 (4)
N3'	-0.1201 (15)	-0.3401 (8)	1.2576 (16)	0.040 (3)	0.158 (4)
O2'	-0.1967 (14)	-0.3283 (7)	1.2810 (14)	0.049 (3)	0.158 (4)
O1'	-0.091 (4)	-0.3889 (11)	1.259 (4)	0.033 (3)	0.158 (4)
Sb	0.035784 (19)	0.195912 (9)	1.342401 (19)	0.03131 (7)	
F1	-0.0552 (2)	0.15895 (13)	1.3963 (3)	0.0868 (9)	
F2	-0.09810 (19)	0.23510 (10)	1.2379 (2)	0.0632 (7)	
F3	0.12724 (18)	0.23192 (9)	1.28696 (18)	0.0447 (5)	
F4	0.0682 (2)	0.25534 (10)	1.4442 (2)	0.0624 (7)	
F5	0.0064 (2)	0.13675 (9)	1.23847 (18)	0.0559 (6)	
F6	0.16940 (18)	0.15634 (9)	1.44683 (17)	0.0461 (5)	

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag	0.01518 (11)	0.01797 (12)	0.02097 (11)	-0.00183 (8)	0.00690 (9)	-0.00001 (9)
P1	0.0148 (3)	0.0175 (4)	0.0195 (4)	-0.0012 (3)	0.0069 (3)	0.0020 (3)
P2	0.0140 (3)	0.0155 (4)	0.0193 (4)	-0.0006 (3)	0.0060 (3)	0.0015 (3)
C21	0.0220 (14)	0.0207 (16)	0.0236 (15)	0.0009 (12)	0.0119 (13)	0.0042 (12)
C22	0.0219 (15)	0.0260 (17)	0.0288 (16)	-0.0009 (13)	0.0141 (13)	0.0049 (13)
C23	0.0249 (16)	0.037 (2)	0.041 (2)	0.0085 (15)	0.0203 (15)	0.0085 (16)
C24	0.044 (2)	0.034 (2)	0.054 (2)	0.0089 (17)	0.0326 (19)	-0.0018 (18)
C25	0.0392 (19)	0.035 (2)	0.045 (2)	-0.0055 (16)	0.0229 (17)	-0.0149 (17)
C26	0.0250 (15)	0.0286 (17)	0.0316 (17)	-0.0025 (14)	0.0142 (14)	-0.0036 (14)
C31	0.0122 (13)	0.0225 (16)	0.0190 (14)	-0.0032 (12)	0.0007 (11)	0.0047 (12)
C32	0.0190 (14)	0.0256 (17)	0.0229 (16)	-0.0019 (13)	0.0027 (13)	0.0019 (13)
C33	0.0229 (16)	0.0212 (17)	0.0294 (17)	-0.0023 (13)	-0.0048 (14)	0.0023 (14)
C34	0.0225 (16)	0.0249 (18)	0.0349 (19)	-0.0070 (14)	-0.0071 (15)	0.0109 (15)
C35	0.0212 (16)	0.043 (2)	0.0323 (18)	-0.0082 (15)	0.0050 (14)	0.0169 (16)
C36	0.0175 (14)	0.0321 (18)	0.0274 (16)	-0.0026 (13)	0.0062 (13)	0.0065 (14)
C41	0.0125 (13)	0.0241 (16)	0.0199 (14)	-0.0032 (12)	0.0047 (12)	0.0002 (12)
C42	0.0230 (15)	0.0291 (18)	0.0303 (17)	0.0016 (13)	0.0125 (14)	0.0067 (14)

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C43	0.0233 (16)	0.043 (2)	0.0299 (17)	-0.0013 (15)	0.0099 (14)	0.0136 (16)
C44	0.0332 (18)	0.052 (2)	0.0255 (17)	-0.0073 (17)	0.0174 (15)	0.0033 (16)
C45	0.0382 (19)	0.038 (2)	0.0373 (19)	-0.0051 (16)	0.0239 (16)	-0.0075 (16)
C46	0.0263 (16)	0.0243 (17)	0.0310 (17)	-0.0030 (13)	0.0161 (14)	0.0007 (13)
C51	0.0165 (13)	0.0235 (16)	0.0209 (15)	0.0007 (12)	0.0080 (12)	0.0062 (12)
C52	0.0208 (15)	0.0215 (17)	0.0403 (19)	-0.0008 (13)	0.0124 (14)	-0.0002 (14)
C53	0.0352 (19)	0.0238 (18)	0.061 (2)	0.0089 (15)	0.0247 (18)	0.0045 (17)
C54	0.0205 (16)	0.043 (2)	0.047 (2)	0.0121 (15)	0.0152 (16)	0.0166 (17)
C55	0.0158 (15)	0.048 (2)	0.0332 (18)	-0.0019 (15)	0.0055 (14)	0.0064 (16)
C56	0.0196 (15)	0.0296 (18)	0.0288 (16)	-0.0015 (13)	0.0108 (13)	-0.0024 (14)
C61	0.0222 (14)	0.0162 (15)	0.0237 (15)	-0.0003 (12)	0.0111 (13)	0.0000 (12)
C1	0.026 (3)	0.029 (3)	0.026 (2)	0.005 (2)	0.0082 (18)	-0.001 (2)
C2	0.047 (3)	0.035 (3)	0.039 (3)	0.012 (3)	0.011 (2)	-0.007 (3)
C3	0.047 (3)	0.021 (2)	0.038 (3)	0.011 (2)	-0.002 (2)	-0.006 (2)
C4	0.028 (3)	0.0185 (19)	0.028 (3)	0.0031 (17)	-0.0086 (17)	0.0019 (18)
C5	0.035 (3)	0.017 (2)	0.037 (4)	-0.007 (2)	-0.015 (2)	0.014 (2)
C6	0.033 (2)	0.039 (3)	0.032 (2)	-0.013 (2)	-0.0048 (18)	0.017 (2)
C7	0.026 (2)	0.040 (3)	0.018 (2)	-0.014 (2)	0.0001 (17)	0.007 (2)
C8	0.034 (3)	0.064 (4)	0.024 (2)	-0.023 (2)	0.0132 (19)	0.002 (2)
C9	0.037 (3)	0.060 (3)	0.033 (2)	-0.018 (2)	0.020 (2)	-0.011 (2)
C10	0.030 (3)	0.042 (3)	0.029 (2)	-0.012 (2)	0.017 (2)	-0.011 (2)
C11	0.016 (2)	0.028 (2)	0.0144 (18)	-0.0046 (17)	-0.0025 (14)	0.0035 (17)
C12	0.020 (2)	0.0213 (18)	0.020 (3)	-0.0026 (16)	-0.0031 (16)	0.0098 (17)
N1	0.019 (3)	0.0228 (18)	0.022 (3)	0.0015 (16)	0.0032 (14)	-0.0027 (16)
N2	0.022 (2)	0.025 (2)	0.0200 (16)	-0.008 (2)	0.0071 (15)	-0.002 (2)
N3	0.038 (2)	0.026 (2)	0.081 (3)	-0.008 (2)	-0.020 (2)	0.018 (2)
O1	0.086 (3)	0.023 (2)	0.269 (8)	0.004 (2)	0.097 (4)	0.008 (3)
O2	0.114 (7)	0.034 (3)	0.066 (5)	-0.031 (3)	-0.016 (3)	0.030 (3)
C1'	0.024 (5)	0.024 (5)	0.023 (5)	0.004 (5)	0.014 (4)	-0.001 (4)
C2'	0.029 (6)	0.025 (6)	0.029 (5)	0.001 (5)	0.016 (5)	0.001 (5)
C3'	0.033 (6)	0.023 (5)	0.030 (6)	0.007 (5)	0.016 (5)	-0.004 (5)
C4'	0.023 (5)	0.020 (4)	0.023 (5)	0.001 (4)	0.007 (4)	0.003 (4)
C5'	0.024 (5)	0.019 (5)	0.025 (6)	-0.004 (5)	0.003 (5)	0.007 (5)
C6'	0.028 (5)	0.028 (5)	0.029 (5)	-0.007 (5)	0.004 (5)	0.010 (5)
C7'	0.021 (4)	0.032 (5)	0.019 (4)	-0.006 (4)	0.004 (4)	0.003 (4)
C8'	0.025 (5)	0.039 (6)	0.023 (5)	-0.011 (5)	0.007 (5)	0.000 (5)
C9'	0.028 (5)	0.046 (5)	0.025 (4)	-0.012 (5)	0.016 (4)	-0.005 (5)
C10'	0.028 (5)	0.037 (5)	0.026 (4)	-0.012 (5)	0.012 (4)	-0.003 (5)
C11'	0.021 (4)	0.022 (4)	0.019 (4)	-0.010 (4)	-0.001 (4)	0.005 (4)
C12'	0.019 (4)	0.022 (4)	0.019 (5)	0.002 (4)	0.004 (4)	-0.001 (4)
N1'	0.020 (5)	0.022 (4)	0.019 (5)	-0.005 (4)	0.009 (4)	0.006 (4)
N2'	0.022 (5)	0.033 (5)	0.017 (4)	-0.008 (5)	0.010 (4)	-0.002 (5)
N3'	0.040 (5)	0.039 (5)	0.043 (5)	-0.007 (5)	0.021 (4)	0.018 (5)
O2'	0.045 (6)	0.043 (6)	0.053 (6)	-0.007 (5)	0.019 (5)	0.020 (5)
O1'	0.039 (5)	0.038 (6)	0.036 (6)	-0.006 (5)	0.030 (5)	0.015 (5)
Sb	0.03320 (12)	0.02695 (13)	0.03999 (14)	0.00654 (9)	0.02232 (11)	0.00912 (10)
F1	0.0786 (18)	0.091 (2)	0.119 (2)	-0.0047 (16)	0.0694 (19)	0.0431 (19)
F2	0.0377 (12)	0.0606 (16)	0.0893 (18)	0.0241 (11)	0.0282 (13)	0.0301 (14)
F3	0.0464 (12)	0.0476 (13)	0.0557 (13)	0.0058 (10)	0.0370 (11)	0.0089 (10)

F4	0.0965 (19)	0.0479 (14)	0.0622 (15)	0.0149 (13)	0.0533 (15)	-0.0061 (12)
F5	0.0565 (14)	0.0377 (12)	0.0437 (13)	0.0067 (11)	-0.0013 (11)	-0.0024 (10)
F6	0.0489 (12)	0.0339 (11)	0.0392 (12)	0.0060 (10)	0.0070 (10)	0.0053 (9)

*Geometric parameters (Å, °)*

Ag—N1	2.392 (6)	C1—N1	1.329 (5)
Ag—P2	2.3982 (7)	C1—C2	1.404 (6)
Ag—N1'	2.38 (3)	C1—H1A	0.9300
Ag—N2'	2.49 (3)	C2—C3	1.353 (7)
Ag—P1	2.4491 (7)	C2—H2A	0.9300
Ag—N2	2.451 (5)	C3—C4	1.403 (7)
P1—C21	1.817 (3)	C3—H3A	0.9300
P1—C31	1.828 (3)	C4—C12	1.437 (5)
P1—C61	1.843 (3)	C4—C5	1.457 (8)
P2—C51	1.821 (3)	C5—C6	1.330 (7)
P2—C41	1.825 (3)	C5—N3	1.483 (6)
P2—C61 <sup>i</sup>	1.835 (3)	C6—C7	1.424 (7)
C21—C26	1.395 (4)	C6—H6A	0.9300
C21—C22	1.398 (4)	C7—C8	1.400 (7)
C22—C23	1.387 (4)	C7—C11	1.408 (5)
C22—H22A	0.9300	C8—C9	1.359 (7)
C23—C24	1.381 (5)	C8—H8A	0.9300
C23—H23A	0.9300	C9—C10	1.395 (6)
C24—C25	1.380 (5)	C9—H9A	0.9300
C24—H24A	0.9300	C10—N2	1.322 (5)
C25—C26	1.383 (4)	C10—H10A	0.9300
C25—H25A	0.9300	C11—N2	1.361 (5)
C26—H26A	0.9300	C11—C12	1.432 (6)
C31—C36	1.395 (4)	C12—N1	1.361 (5)
C31—C32	1.396 (4)	N3—O2	1.191 (8)
C32—C33	1.385 (4)	N3—O1	1.198 (7)
C32—H32A	0.9300	C1'—N1'	1.325 (17)
C33—C34	1.382 (5)	C1'—C2'	1.405 (17)
C33—H33A	0.9300	C1'—H1'A	0.9300
C34—C35	1.376 (5)	C2'—C3'	1.350 (18)
C34—H34A	0.9300	C2'—H2'A	0.9300
C35—C36	1.388 (4)	C3'—C4'	1.397 (17)
C35—H35A	0.9300	C3'—H3'A	0.9300
C36—H36A	0.9300	C4'—C12'	1.440 (16)
C41—C46	1.383 (4)	C4'—C5'	1.447 (17)
C41—C42	1.400 (4)	C5'—C6'	1.322 (19)
C42—C43	1.384 (4)	C5'—H5'A	0.9300
C42—H42A	0.9300	C6'—C7'	1.435 (18)
C43—C44	1.379 (5)	C6'—N3'	1.50 (3)
C43—H43A	0.9300	C7'—C8'	1.387 (17)
C44—C45	1.376 (5)	C7'—C11'	1.429 (16)
C44—H44A	0.9300	C8'—C9'	1.357 (18)
C45—C46	1.396 (4)	C8'—H8'A	0.9300

## supplementary materials

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C45—H45A	0.9300	C9'—C10'	1.417 (17)
C46—H46A	0.9300	C9'—H9'A	0.9300
C51—C52	1.386 (4)	C10'—N2'	1.324 (17)
C51—C56	1.394 (4)	C10'—H10B	0.9300
C52—C53	1.392 (4)	C11'—N2'	1.349 (16)
C52—H52A	0.9300	C11'—C12'	1.420 (16)
C53—C54	1.376 (5)	C12'—N1'	1.354 (16)
C53—H53A	0.9300	N3'—O2'	1.197 (16)
C54—C55	1.372 (5)	N3'—O1'	1.197 (19)
C54—H54A	0.9300	Sb—F1	1.853 (2)
C55—C56	1.390 (4)	Sb—F3	1.8630 (19)
C55—H55A	0.9300	Sb—F4	1.864 (2)
C56—H56A	0.9300	Sb—F2	1.874 (2)
C61—P2 <sup>i</sup>	1.835 (3)	Sb—F6	1.8759 (19)
C61—H61A	0.9700	Sb—F5	1.883 (2)
C61—H61B	0.9700		
N1—Ag—P2	115.8 (3)	N1—C1—C2	122.1 (5)
N1—Ag—N1'	6.2 (7)	N1—C1—H1A	119.0
P2—Ag—N1'	113.8 (17)	C2—C1—H1A	119.0
N1—Ag—N2'	62.3 (6)	C3—C2—C1	119.4 (5)
P2—Ag—N2'	104.1 (13)	C3—C2—H2A	120.3
N1'—Ag—N2'	68.3 (7)	C1—C2—H2A	120.3
N1—Ag—P1	100.1 (3)	C2—C3—C4	120.7 (4)
P2—Ag—P1	144.11 (3)	C2—C3—H3A	119.6
N1'—Ag—P1	101.7 (17)	C4—C3—H3A	119.6
N2—Ag—P1	93.4 (14)	C3—C4—C12	117.1 (4)
N1—Ag—N2	68.51 (15)	C3—C4—C5	127.6 (4)
P2—Ag—N2	103.1 (2)	C12—C4—C5	115.2 (5)
N1'—Ag—N2	74.5 (6)	C6—C5—C4	123.5 (4)
N2—Ag—N2	6.3 (7)	C6—C5—N3	115.5 (6)
P1—Ag—N2	90.9 (2)	C4—C5—N3	121.0 (6)
C21—P1—C31	106.38 (13)	C5—C6—C7	121.5 (5)
C21—P1—C61	105.11 (13)	C5—C6—H6A	119.2
C31—P1—C61	102.66 (13)	C7—C6—H6A	119.2
C21—P1—Ag	113.91 (10)	C8—C7—C11	118.9 (4)
C31—P1—Ag	105.39 (9)	C8—C7—C6	122.7 (4)
C61—P1—Ag	121.90 (9)	C11—C7—C6	118.4 (5)
C51—P2—C41	101.49 (13)	C9—C8—C7	118.9 (4)
C51—P2—C61 <sup>i</sup>	104.48 (13)	C9—C8—H8A	120.5
C41—P2—C61 <sup>i</sup>	104.99 (13)	C7—C8—H8A	120.5
C51—P2—Ag	119.29 (10)	C8—C9—C10	119.0 (5)
C41—P2—Ag	106.43 (9)	C8—C9—H9A	120.5
C61 <sup>i</sup> —P2—Ag	118.08 (10)	C10—C9—H9A	120.5
C26—C21—C22	118.7 (3)	N2—C10—C9	123.8 (5)
C26—C21—P1	118.7 (2)	N2—C10—H10A	118.1
C22—C21—P1	122.5 (2)	C9—C10—H10A	118.1
C23—C22—C21	120.1 (3)	N2—C11—C7	121.3 (4)
C23—C22—H22A	119.9	N2—C11—C12	118.2 (4)

C21—C22—H22A	119.9	C7—C11—C12	120.5 (4)
C24—C23—C22	120.2 (3)	N1—C12—C4	120.8 (5)
C24—C23—H23A	119.9	N1—C12—C11	118.5 (4)
C22—C23—H23A	119.9	C4—C12—C11	120.7 (4)
C25—C24—C23	120.4 (3)	C1—N1—C12	119.8 (4)
C25—C24—H24A	119.8	C1—N1—Ag	121.8 (4)
C23—C24—H24A	119.8	C12—N1—Ag	118.1 (3)
C24—C25—C26	119.7 (3)	C10—N2—C11	118.0 (4)
C24—C25—H25A	120.1	C10—N2—Ag	125.2 (3)
C26—C25—H25A	120.1	C11—N2—Ag	116.0 (3)
C25—C26—C21	120.9 (3)	O2—N3—O1	122.8 (6)
C25—C26—H26A	119.5	O2—N3—C5	118.7 (7)
C21—C26—H26A	119.5	O1—N3—C5	118.6 (6)
C36—C31—C32	118.9 (3)	N1'—C1'—C2'	122 (2)
C36—C31—P1	122.0 (2)	N1'—C1'—H1'A	119.1
C32—C31—P1	118.4 (2)	C2'—C1'—H1'A	119.1
C33—C32—C31	120.7 (3)	C3'—C2'—C1'	119 (2)
C33—C32—H32A	119.6	C3'—C2'—H2'A	120.3
C31—C32—H32A	119.6	C1'—C2'—H2'A	120.3
C34—C33—C32	119.6 (3)	C2'—C3'—C4'	120.9 (19)
C34—C33—H33A	120.2	C2'—C3'—H3'A	119.6
C32—C33—H33A	120.2	C4'—C3'—H3'A	119.6
C35—C34—C33	120.4 (3)	C3'—C4'—C12'	117.0 (16)
C35—C34—H34A	119.8	C3'—C4'—C5'	126.3 (18)
C33—C34—H34A	119.8	C12'—C4'—C5'	116.6 (16)
C34—C35—C36	120.5 (3)	C6'—C5'—C4'	123 (2)
C34—C35—H35A	119.8	C6'—C5'—H5'A	118.7
C36—C35—H35A	119.8	C4'—C5'—H5'A	118.7
C35—C36—C31	119.9 (3)	C5'—C6'—C7'	122 (2)
C35—C36—H36A	120.1	C5'—C6'—N3'	115.7 (19)
C31—C36—H36A	120.1	C7'—C6'—N3'	121.9 (18)
C46—C41—C42	118.8 (3)	C8'—C7'—C6'	124.6 (17)
C46—C41—P2	123.7 (2)	C8'—C7'—C11'	117.2 (16)
C42—C41—P2	117.3 (2)	C6'—C7'—C11'	117.6 (17)
C43—C42—C41	120.5 (3)	C9'—C8'—C7'	121.4 (18)
C43—C42—H42A	119.7	C9'—C8'—H8'A	119.3
C41—C42—H42A	119.7	C7'—C8'—H8'A	119.3
C44—C43—C42	120.0 (3)	C8'—C9'—C10'	118.9 (18)
C44—C43—H43A	120.0	C8'—C9'—H9'A	120.5
C42—C43—H43A	120.0	C10'—C9'—H9'A	120.5
C45—C44—C43	120.1 (3)	N2'—C10'—C9'	121 (2)
C45—C44—H44A	119.9	N2'—C10'—H10B	119.7
C43—C44—H44A	119.9	C9'—C10'—H10B	119.7
C44—C45—C46	120.2 (3)	N2'—C11'—C7'	120.3 (17)
C44—C45—H45A	119.9	N2'—C11'—C12'	119.5 (16)
C46—C45—H45A	119.9	C7'—C11'—C12'	120.0 (17)
C41—C46—C45	120.3 (3)	N1'—C12'—C4'	120.5 (17)
C41—C46—H46A	119.8	N1'—C12'—C11'	118.7 (17)
C45—C46—H46A	119.8	C4'—C12'—C11'	120.3 (17)

## supplementary materials

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C52—C51—C56	119.3 (3)	C1'—N1'—C12'	120 (2)
C52—C51—P2	120.1 (2)	C1'—N1'—Ag	121.4 (17)
C56—C51—P2	120.6 (2)	C12'—N1'—Ag	117.8 (15)
C51—C52—C53	120.3 (3)	C10'—N2'—C11'	121.4 (19)
C51—C52—H52A	119.9	C10'—N2'—Ag	124.1 (16)
C53—C52—H52A	119.9	C11'—N2'—Ag	114.3 (14)
C54—C53—C52	119.8 (3)	O2'—N3'—O1'	120.1 (19)
C54—C53—H53A	120.1	O2'—N3'—C6'	118.5 (18)
C52—C53—H53A	120.1	O1'—N3'—C6'	121 (2)
C55—C54—C53	120.4 (3)	F1—Sb—F3	179.02 (13)
C55—C54—H54A	119.8	F1—Sb—F4	91.09 (13)
C53—C54—H54A	119.8	F3—Sb—F4	89.86 (10)
C54—C55—C56	120.3 (3)	F1—Sb—F2	90.32 (12)
C54—C55—H55A	119.8	F3—Sb—F2	89.92 (10)
C56—C55—H55A	119.8	F4—Sb—F2	90.14 (12)
C55—C56—C51	119.8 (3)	F1—Sb—F6	89.50 (11)
C55—C56—H56A	120.1	F3—Sb—F6	90.25 (9)
C51—C56—H56A	120.1	F4—Sb—F6	90.09 (10)
P2 <sup>i</sup> —C61—P1	112.26 (15)	F2—Sb—F6	179.72 (11)
P2 <sup>i</sup> —C61—H61A	109.2	F1—Sb—F5	90.56 (14)
P1—C61—H61A	109.2	F3—Sb—F5	88.49 (10)
P2 <sup>i</sup> —C61—H61B	109.2	F4—Sb—F5	178.33 (11)
P1—C61—H61B	109.2	F2—Sb—F5	90.13 (11)
H61A—C61—H61B	107.9	F6—Sb—F5	89.65 (9)
N1—Ag—P1—C21	143.06 (17)	C61 <sup>i</sup> —P2—C51—C56	46.3 (3)
P2—Ag—P1—C21	−39.37 (11)	Ag—P2—C51—C56	−179.1 (2)
N1'—Ag—P1—C21	149.1 (6)	C56—C51—C52—C53	−0.9 (5)
N2'—Ag—P1—C21	80.6 (6)	P2—C51—C52—C53	−178.5 (3)
N2—Ag—P1—C21	74.73 (15)	C51—C52—C53—C54	0.3 (5)
N1—Ag—P1—C31	26.83 (17)	C52—C53—C54—C55	−0.3 (5)
P2—Ag—P1—C31	−155.60 (10)	C53—C54—C55—C56	1.0 (5)
N1'—Ag—P1—C31	32.9 (6)	C54—C55—C56—C51	−1.6 (5)
N2'—Ag—P1—C31	−35.7 (6)	C52—C51—C56—C55	1.6 (4)
N2—Ag—P1—C31	−41.50 (15)	P2—C51—C56—C55	179.2 (2)
N1—Ag—P1—C61	−89.21 (17)	C21—P1—C61—P2 <sup>i</sup>	49.57 (18)
P2—Ag—P1—C61	88.35 (12)	C31—P1—C61—P2 <sup>i</sup>	160.67 (15)
N1'—Ag—P1—C61	−83.2 (6)	Ag—P1—C61—P2 <sup>i</sup>	−81.92 (16)
N2'—Ag—P1—C61	−151.7 (6)	C2—C1—N1—Ag	−174.5 (6)
N2—Ag—P1—C61	−157.54 (15)	C4—C12—N1—Ag	174.2 (5)
N1—Ag—P2—C51	24.36 (19)	C11—C12—N1—Ag	−3.4 (11)
N1'—Ag—P2—C51	17.9 (7)	P2—Ag—N1—C1	−85.9 (8)
N2'—Ag—P2—C51	90.1 (8)	N1'—Ag—N1—C1	−14 (18)
P1—Ag—P2—C51	−152.97 (11)	N2'—Ag—N1—C1	−178.9 (18)
N2—Ag—P2—C51	96.58 (17)	P1—Ag—N1—C1	92.5 (8)
N1—Ag—P2—C41	−89.44 (18)	N2—Ag—N1—C1	179.5 (9)
N1'—Ag—P2—C41	−95.8 (7)	P2—Ag—N1—C12	100.1 (7)
N2—Ag—P2—C41	−23.7 (8)	N1'—Ag—N1—C12	172 (19)

P1—Ag—P2—C41	93.23 (11)	N2'—Ag—N1—C12	7.1 (17)
N2—Ag—P2—C41	-17.21 (16)	P1—Ag—N1—C12	-81.5 (8)
N1—Ag—P2—C61 <sup>i</sup>	152.98 (18)	N2—Ag—N1—C12	5.5 (7)
N1'—Ag—P2—C61 <sup>i</sup>	146.6 (7)	C9—C10—N2—C11	-0.7 (11)
N2'—Ag—P2—C61 <sup>i</sup>	-141.2 (8)	C9—C10—N2—Ag	168.8 (5)
P1—Ag—P2—C61 <sup>i</sup>	-24.35 (12)	C7—C11—N2—C10	-0.9 (11)
N2—Ag—P2—C61 <sup>i</sup>	-134.79 (17)	C12—C11—N2—C10	178.9 (7)
C31—P1—C21—C26	133.8 (2)	C7—C11—N2—Ag	-171.3 (5)
C61—P1—C21—C26	-117.8 (2)	C12—C11—N2—Ag	8.5 (9)
Ag—P1—C21—C26	18.2 (3)	N1—Ag—N2—C10	-176.9 (8)
C31—P1—C21—C22	-49.0 (3)	P2—Ag—N2—C10	70.2 (7)
C61—P1—C21—C22	59.4 (3)	N1'—Ag—N2—C10	-178.3 (19)
Ag—P1—C21—C22	-164.7 (2)	N2'—Ag—N2—C10	170 (15)
C26—C21—C22—C23	1.1 (4)	P1—Ag—N2—C10	-76.4 (7)
P1—C21—C22—C23	-176.0 (2)	N1—Ag—N2—C11	-7.2 (6)
C21—C22—C23—C24	-1.2 (5)	P2—Ag—N2—C11	-120.1 (6)
C22—C23—C24—C25	0.5 (5)	N1'—Ag—N2—C11	-8.7 (18)
C23—C24—C25—C26	0.3 (6)	N2'—Ag—N2—C11	-20 (14)
C24—C25—C26—C21	-0.4 (5)	P1—Ag—N2—C11	93.2 (6)
C22—C21—C26—C25	-0.3 (5)	C6—C5—N3—O2	-6.1 (8)
P1—C21—C26—C25	176.9 (3)	C4—C5—N3—O2	171.9 (7)
C21—P1—C31—C36	-27.8 (3)	C6—C5—N3—O1	174.2 (5)
C61—P1—C31—C36	-138.0 (2)	C4—C5—N3—O1	-7.8 (7)
Ag—P1—C31—C36	93.5 (2)	N1—Ag—N1'—C1'	169 (23)
C21—P1—C31—C32	161.8 (2)	P2—Ag—N1'—C1'	-81 (5)
C61—P1—C31—C32	51.7 (2)	N2'—Ag—N1'—C1'	-177 (5)
Ag—P1—C31—C32	-76.9 (2)	P1—Ag—N1'—C1'	94 (5)
C36—C31—C32—C33	-1.3 (4)	N2—Ag—N1'—C1'	-179 (5)
P1—C31—C32—C33	169.4 (2)	N1—Ag—N1'—C12'	-3(15)
C31—C32—C33—C34	0.3 (4)	P2—Ag—N1'—C12'	107 (4)
C32—C33—C34—C35	0.8 (4)	N2'—Ag—N1'—C12'	10 (4)
C33—C34—C35—C36	-0.9 (5)	P1—Ag—N1'—C12'	-79 (5)
C34—C35—C36—C31	-0.1 (4)	N2—Ag—N1'—C12'	9(4)
C32—C31—C36—C35	1.2 (4)	C9'—C10'—N2'—C11'	-4(7)
P1—C31—C36—C35	-169.2 (2)	C9'—C10'—N2'—Ag	171 (3)
C51—P2—C41—C46	135.8 (2)	C7'—C11'—N2'—C10'	6(7)
C61 <sup>i</sup> —P2—C41—C46	27.2 (3)	C12'—C11'—N2'—C10'	-179 (5)
Ag—P2—C41—C46	-98.7 (2)	C7'—C11'—N2'—Ag	-169 (3)
C51—P2—C41—C42	-48.9 (2)	C12'—C11'—N2'—Ag	6(6)
C61 <sup>i</sup> —P2—C41—C42	-157.5 (2)	N1—Ag—N2'—C10'	178 (5)
Ag—P2—C41—C42	76.5 (2)	P2—Ag—N2'—C10'	66 (4)
C46—C41—C42—C43	-0.5 (4)	N1'—Ag—N2'—C10'	177 (5)
P2—C41—C42—C43	-176.0 (2)	P1—Ag—N2'—C10'	-82 (4)
C41—C42—C43—C44	-0.7 (5)	N2—Ag—N2'—C10'	-15 (11)
C42—C43—C44—C45	1.2 (5)	N1—Ag—N2'—C11'	-7(3)
C43—C44—C45—C46	-0.4 (5)	P2—Ag—N2'—C11'	-119 (4)
C42—C41—C46—C45	1.3 (4)	N1'—Ag—N2'—C11'	-8(4)

## supplementary materials

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P2—C41—C46—C45	176.5 (2)	P1—Ag—N2'—C11'	93 (4)
C44—C45—C46—C41	-0.8 (5)	N2—Ag—N2'—C11'	160 (17)
C41—P2—C51—C52	114.9 (3)	C5'—C6'—N3'—O2'	-156 (3)
C61 <sup>i</sup> —P2—C51—C52	-136.2 (2)	C7'—C6'—N3'—O2'	23 (4)
Ag—P2—C51—C52	-1.6 (3)	C5'—C6'—N3'—O1'	16 (5)
C41—P2—C51—C56	-62.7 (3)	C7'—C6'—N3'—O1'	-166 (4)

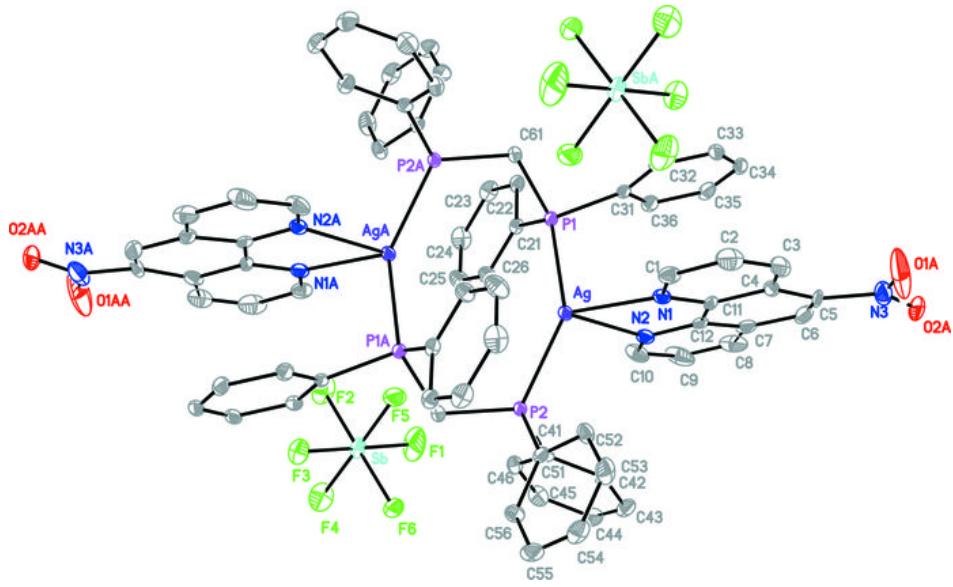
Symmetry codes: (i)  $-x, -y, -z+2$ .

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

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
C35—H35A…F4 <sup>ii</sup>	0.93	2.54	3.409 (4)	155
C46—H46A…F5	0.93	2.50	3.398 (4)	163

Symmetry codes: (ii)  $-x-1/2, y-1/2, -z+5/2$ .

**Fig. 1**



## **supplementary materials**

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**Fig. 2**

