

Acta Crystallographica Section E

**Structure Reports**

**Online**

ISSN 1600-5368

Editors: **W. Clegg** and **D. G. Watson**

**(*P*)-Tetra- $\mu_3$ -iodido-tetrakis[(cyclohexyldiphenylphosphine- $\kappa P$ )silver(I)]**

**John F. Young and Glenn P. A. Yap**

Copyright © International Union of Crystallography

Author(s) of this paper may load this reprint on their own web site or institutional repository provided that this cover page is retained. Republication of this article or its storage in electronic databases other than as specified above is not permitted without prior permission in writing from the IUCr.

For further information see <http://journals.iucr.org/services/authorrights.html>

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

**(P)-Tetra- $\mu_3$ -iodido-tetrakis[(cyclohexyl-diphenylphosphine- $\kappa P$ )]silver(I)**

John F. Young and Glenn P. A. Yap\*

Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, USA

Correspondence e-mail: gpyap@udel.edu

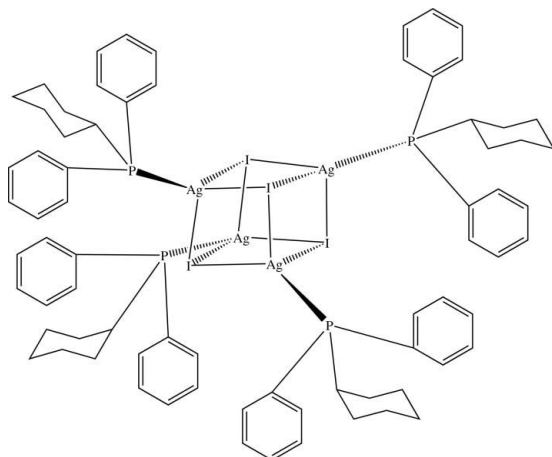
Received 14 June 2007; accepted 29 June 2007

Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(\text{C}-\text{C}) = 0.012$  Å; disorder in main residue;  $R$  factor = 0.043;  $wR$  factor = 0.107; data-to-parameter ratio = 22.9.

The title compound,  $[\text{Ag}_4\text{I}_4(\text{C}_{18}\text{H}_{21}\text{P})_4]$ , has a tetrameric structure, with the Ag and I atoms alternating in a distorted cubane-like AgI core and with cyclohexyldiphenylphosphine ligands capping the Ag corners. Each face is distorted, such that the average  $\text{Ag}\cdots\text{Ag}$  atomic separation is shorter than the average  $\text{I}\cdots\text{I}$  atomic separation by about 1 Å. Two symmetry-unique but structurally similar tetramers of the same enantiomer are each located on a twofold rotation axis, which can be assigned the same helicity, suggesting spontaneous resolution. Three phenyl groups are each disordered over two positions; the site occupancy ratios are between *ca* 2:1 and 4:1.

## Related literature

Background information on similar tetrameric AgI monodentate adducts is given by Bowen *et al.* (1994), Teo & Calabrese (1975, 1976) and Meijboom *et al.* (2006). A background reference on helicity is Eliel *et al.* (1994).



## Experimental

## Crystal data

$[\text{Ag}_4\text{I}_4(\text{C}_{18}\text{H}_{21}\text{P})_4]$   
 $M_r = 2012.35$   
 Monoclinic,  $C2$   
 $a = 24.698$  (9) Å  
 $b = 12.404$  (5) Å  
 $c = 24.328$  (9) Å  
 $\beta = 104.145$  (7)°

$V = 7227$  (5) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.91$  mm<sup>-1</sup>  
 $T = 120$  (2) K  
 $0.15 \times 0.14 \times 0.09$  mm

## Data collection

Bruker APEX diffractometer  
 Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2002)  
 $T_{\min} = 0.652$ ,  $T_{\max} = 0.767$

42119 measured reflections  
 16990 independent reflections  
 15397 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.041$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.107$   
 $S = 1.05$   
 16990 reflections  
 742 parameters  
 327 restraints

H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 2.48$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.26$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 with 7870 Friedel pairs  
 Flack parameter:  $-0.029$  (18)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

The authors thank Professor Klaus H. Theopold, Director of the Center for Catalytic Science and Technology, for synthetic assistance, the Department of Chemistry and Biochemistry for the purchase of reagents, and Professors Joseph M. Fox and Douglass F. Taber for discussions on helicity.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2128).

## References

- Bowen, R. J., Camp, D., Effendy, Healy, P. C., Skelton, B. W. & White, A. H. (1994). *Aust. J. Chem.* **47**, 693–701.  
 Bruker (2002). *SMART* (Version 5.62), *SAINT* (Version 6.02), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Eliel, E. L., Wilen, S. H. & Mander, L. N. (1994). *Stereochemistry of Organic Compounds*. New York: Wiley-Interscience.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Meijboom, R., Muller, A. & Roodt, A. (2006). *Acta Cryst.* **E62**, m2162–m2164.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
 Teo, B.-K. & Calabrese, J. C. (1975). *J. Am. Chem. Soc.* **97**, 1256–1257.  
 Teo, B.-K. & Calabrese, J. C. (1976). *Inorg. Chem.* **15**, 2474–2486.

## **supplementary materials**

*Acta Cryst.* (2007). E63, m2075 [ doi:10.1107/S1600536807031911 ]

**(P)-Tetra- $\mu_3$ -iodido-tetrakis[(cyclohexyldiphenylphosphine- $\mu_3$ -P)silver(I)]**

**J. F. Young and G. P. A. Yap**

**Comment**

The 1:1 AgI:PCyPh<sub>2</sub> (PCyPh<sub>2</sub> is diphenylcyclohexylphosphine) tetrameric complex is similar to reported analogues with other monodentate phosphine ligands (Bowen *et al.*, 1994; Teo & Calabrese, 1975 and 1976; Meijboom *et al.*, 2006). The silver and iodine atoms alternate in a distorted cubane-like AgI core with phosphine capping the silver corners (Fig. 1). Two symmetry unique but structurally similar tetramers are each located on a twofold axis. Each face is distorted such that the average Ag...Ag atomic separation is shorter than the average I...I atomic separation by about 1 Å. A closer inspection shows that the two faces completed by the twofold axis differ from each other and from the four adjacent faces in that they display the shortest and longest I...I separations for each cubane. If the face with the shortest I...I separation is assigned to be proximal, an inspection of the cyclohexyl fragments clearly show (P) helicity (Elieil *et al.*, 1994) for both symmetry unique molecules (Fig. 2). The starting materials do not display chirality suggesting spontaneous resolution during crystallization. We also note that the proximal and distal planes could easily be inverted by slight distortion of the cubane-like core. Alternatively, concerted rotation along the Ag—P bonds would reverse the helicity. The Flack parameter refined to a value of -0.029 (18) indicating the true hand of the data has been correctly determined.

**Experimental**

Synthesis of [Ag(PCyPh<sub>2</sub>)I]<sub>4</sub>: 1 equivalent of AgI and 1.1 equivalents of diphenylcyclohexylphosphine were added in vial containing anhydrous tetrahydrofuran (THF). The mixture was allowed to stir for 3 h at room temperature in darkness. Removal of THF yielded a white powder residue which was washed with several portions of pentane. Colorless crystals were grown by layering pentane over a saturated CH<sub>2</sub>Cl<sub>2</sub> solution at room temperature in the dark (yield 50%).

**Refinement**

Three symmetry unique phenyl groups in [Ag(PCyPh<sub>2</sub>)I]<sub>4</sub> were located disordered each in two positions and were treated as rigid flat hexagons having C—C distances constrained to 1.39 Å with refined site occupancies of 67/33, 70/30 and 78/22, respectively, and were subjected to rigid bond restraints. Equal atomic displacement parameters were applied to chemically equivalent atoms in the disordered contributions and bond distances were restrained to be the same. An anti-bumping restraint was applied between C64, a carbon atom of a minor disordered contributor, and C39 in a cyclohexyl ring. H atoms were assigned calculated positions with  $U_{iso}$  restrained to be 1.2 $U_{eq}$  of the bonded C atom and a C—H distance of 0.95–0.99 Å. The highest peak and deepest hole in the final difference map are located 0.97 and 0.72 Å, respectively, from Ag1.

## supplementary materials

### Figures

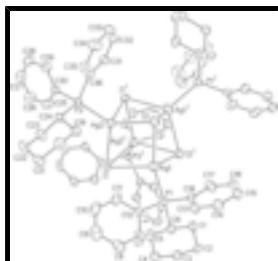


Fig. 1. Diagram showing the molecular structure of the 1:1 AgI:PCyPh<sub>2</sub> tetrameric complex with ellipsoids drawn at the 30% probability level. A second unique but similar molecule of the title compound, the minor disordered components, and the H atoms are omitted for clarity. [Symmetry operator: i)  $-x + 1, y, -z + 1.$ ]

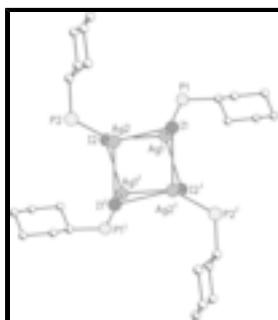


Fig. 2. Abbreviated diagram of the title compound showing (P) helicity of the PCy fragments viewed down the twofold axis with Ag—I—Ag—I face of the shortest I...I distance selected to be proximal. [Symmetry operator: i)  $-x + 1, y, -z + 1.$ ]

### (P)-Tetra- $\mu_3$ -iodido-tetrakis[(cyclohexyldiphenylphosphine- $\kappa P$ )]silver(I)]

#### Crystal data

[Ag<sub>4</sub>I<sub>4</sub>(C<sub>18</sub>H<sub>21</sub>P)<sub>4</sub>]

$M_r = 2012.35$

Monoclinic, C2

Hall symbol: C 2y

$a = 24.698$  (9) Å

$b = 12.404$  (5) Å

$c = 24.328$  (9) Å

$\beta = 104.145$  (7)°

$V = 7227$  (5) Å<sup>3</sup>

$Z = 4$

$F_{000} = 3904$

$D_x = 1.849$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 998 reflections

$\theta = 2.4$ – $26.6$ °

$\mu = 2.91$  mm<sup>-1</sup>

$T = 120$  (2) K

Block, colourless

$0.15 \times 0.14 \times 0.09$  mm

#### Data collection

Bruker APEX  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 120$ (2) K

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2002)

$T_{\min} = 0.652, T_{\max} = 0.767$

16990 independent reflections

15397 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\text{max}} = 28.3$ °

$\theta_{\text{min}} = 1.7$ °

$h = -32 \rightarrow 32$

$k = -16 \rightarrow 16$

42119 measured reflections

$l = -31 \rightarrow 32$

### Refinement

Refinement on  $F^2$

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.043$

$$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 26.0708P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.107$

$(\Delta/\sigma)_{\max} = 0.002$

$S = 1.05$

$\Delta\rho_{\max} = 2.48 \text{ e } \text{\AA}^{-3}$

16990 reflections

$\Delta\rho_{\min} = -1.26 \text{ e } \text{\AA}^{-3}$

742 parameters

Extinction correction: none

327 restraints

Absolute structure: Flack (1983), 7870 Friedel pairs

Primary atom site location: structure-invariant direct methods

Flack parameter:  $-0.029$  (18)

Secondary atom site location: difference Fourier map

### Special details

**Experimental.** Data collection is performed with four batch runs at  $\varphi = 0.00^\circ$  (600 frames), at  $\varphi = 90.00^\circ$  (600 frames), at  $\varphi = 180^\circ$  (600 frames) and at  $\varphi = 270^\circ$  (600 frames). Frame width =  $0.30^\circ$  in  $\omega$ . Data is merged, corrected for decay, and treated with multi-scan absorption corrections.

**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  $F^2 > 2\sigma(F^2)$  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)
Ag1	0.57326 (3)	0.94301 (5)	0.52831 (3)	0.06118 (18)	
Ag2	0.49338 (3)	0.74512 (5)	0.57164 (2)	0.04812 (14)	
Ag3	1.01975 (3)	0.55462 (5)	0.07637 (3)	0.05755 (17)	
Ag4	0.93112 (2)	0.35289 (4)	0.00325 (3)	0.04431 (13)	
I1	0.591930 (19)	0.70934 (4)	0.53562 (2)	0.04137 (11)	
I2	0.48125 (2)	0.97682 (4)	0.58617 (2)	0.05396 (13)	
I3	0.90958 (2)	0.58414 (3)	0.00354 (2)	0.04997 (13)	
I4	1.027377 (18)	0.32713 (3)	0.098437 (18)	0.03722 (9)	
P1	0.65521 (8)	1.04838 (16)	0.57606 (8)	0.0425 (4)	
P2	0.46790 (7)	0.64854 (14)	0.64952 (7)	0.0333 (3)	
P3	1.04524 (11)	0.66022 (16)	0.16369 (9)	0.0521 (5)	
P4	0.84888 (7)	0.24331 (15)	0.00446 (7)	0.0372 (4)	

## supplementary materials

---

C1	0.6946 (3)	1.1312 (6)	0.4848 (3)	0.0504 (18)	
H1A	0.6815	1.2028	0.4941	0.060*	
H1B	0.6633	1.0954	0.4577	0.060*	
C2	0.7433 (3)	1.1453 (6)	0.4577 (4)	0.056 (2)	
H2A	0.7732	1.1868	0.4837	0.067*	
H2B	0.7309	1.1870	0.4222	0.067*	
C3	0.7666 (4)	1.0373 (7)	0.4447 (4)	0.055 (2)	
H3A	0.7382	0.9995	0.4152	0.066*	
H3B	0.7999	1.0496	0.4296	0.066*	
C4	0.7824 (4)	0.9681 (8)	0.4965 (4)	0.063 (2)	
H4A	0.8144	1.0010	0.5239	0.076*	
H4B	0.7941	0.8962	0.4860	0.076*	
C5	0.7329 (4)	0.9549 (6)	0.5246 (4)	0.055 (2)	
H5A	0.7024	0.9144	0.4989	0.066*	
H5B	0.7452	0.9131	0.5602	0.066*	
C6	0.7114 (3)	1.0649 (6)	0.5376 (3)	0.0465 (17)	
H6A	0.7431	1.1030	0.5638	0.056*	
C7	0.7451 (7)	1.0293 (11)	0.6723 (6)	0.049 (3)	0.67 (4)
H7A	0.7581	1.0949	0.6599	0.059*	0.67 (4)
C8	0.7783 (4)	0.9733 (16)	0.7177 (6)	0.065 (3)	0.67 (4)
H8A	0.8140	1.0007	0.7364	0.078*	0.67 (4)
C9	0.7593 (8)	0.8773 (13)	0.7358 (6)	0.084 (5)	0.67 (4)
H9A	0.7820	0.8391	0.7668	0.101*	0.67 (4)
C10	0.7071 (10)	0.8373 (14)	0.7084 (7)	0.091 (6)	0.67 (4)
H10A	0.6942	0.7717	0.7208	0.109*	0.67 (4)
C11	0.6739 (7)	0.8933 (16)	0.6630 (7)	0.073 (5)	0.67 (4)
H11A	0.6383	0.8659	0.6443	0.088*	0.67 (4)
C12	0.6929 (6)	0.9892 (11)	0.6449 (5)	0.048 (2)	0.67 (4)
C73	0.7553 (11)	1.002 (3)	0.6688 (12)	0.049 (3)	0.33 (4)
H73A	0.7789	1.0477	0.6534	0.059*	0.33 (4)
C74	0.7773 (10)	0.944 (3)	0.7179 (13)	0.065 (3)	0.33 (4)
H74A	0.8159	0.9494	0.7361	0.078*	0.33 (4)
C75	0.7428 (18)	0.877 (3)	0.7405 (12)	0.084 (5)	0.33 (4)
H75A	0.7579	0.8376	0.7741	0.101*	0.33 (4)
C76	0.6864 (17)	0.869 (3)	0.7139 (16)	0.091 (6)	0.33 (4)
H76A	0.6628	0.8241	0.7293	0.109*	0.33 (4)
C77	0.6644 (11)	0.928 (3)	0.6647 (15)	0.073 (5)	0.33 (4)
H77A	0.6258	0.9224	0.6465	0.088*	0.33 (4)
C78	0.6989 (12)	0.994 (2)	0.6422 (10)	0.048 (2)	0.33 (4)
C13	0.6649 (4)	1.2421 (7)	0.6414 (4)	0.056 (2)	
H13A	0.6908	1.2052	0.6707	0.067*	
C14	0.6532 (4)	1.3491 (7)	0.6486 (4)	0.056 (2)	
H14A	0.6694	1.3842	0.6834	0.068*	
C15	0.6181 (4)	1.4050 (7)	0.6054 (4)	0.054 (2)	
H15A	0.6113	1.4795	0.6097	0.065*	
C16	0.5931 (4)	1.3525 (7)	0.5562 (4)	0.058 (2)	
H16A	0.5688	1.3911	0.5265	0.069*	
C17	0.6029 (4)	1.2434 (8)	0.5491 (4)	0.058 (2)	
H17A	0.5845	1.2074	0.5152	0.069*	

## supplementary materials

C18	0.6396 (3)	1.1876 (6)	0.5920 (3)	0.0392 (15)
C19	0.5484 (3)	0.7426 (6)	0.7368 (4)	0.0514 (18)
H19A	0.5196	0.7974	0.7382	0.062*
H19B	0.5691	0.7669	0.7090	0.062*
C20	0.5890 (4)	0.7326 (7)	0.7957 (4)	0.056 (2)
H20A	0.6095	0.8013	0.8054	0.068*
H20B	0.5674	0.7194	0.8245	0.068*
C21	0.6300 (3)	0.6427 (8)	0.7976 (4)	0.057 (2)
H21A	0.6561	0.6628	0.7743	0.068*
H21B	0.6521	0.6333	0.8372	0.068*
C22	0.6030 (4)	0.5390 (7)	0.7768 (4)	0.059 (2)
H22A	0.5817	0.5125	0.8037	0.071*
H22B	0.6321	0.4850	0.7754	0.071*
C23	0.5634 (4)	0.5501 (7)	0.7177 (4)	0.058 (2)
H23A	0.5851	0.5697	0.6899	0.069*
H23B	0.5448	0.4801	0.7061	0.069*
C24	0.5200 (3)	0.6348 (5)	0.7175 (3)	0.0374 (14)
H24A	0.4994	0.6130	0.7464	0.045*
C25	0.4719 (4)	0.4442 (7)	0.6074 (4)	0.057 (2)
H25A	0.5020	0.4733	0.5942	0.068*
C26	0.4587 (4)	0.3355 (8)	0.5979 (4)	0.065 (2)
H26A	0.4807	0.2907	0.5803	0.078*
C27	0.4141 (4)	0.2941 (7)	0.6140 (4)	0.061 (2)
H27A	0.4053	0.2197	0.6086	0.074*
C28	0.3817 (4)	0.3604 (8)	0.6382 (4)	0.066 (2)
H28A	0.3492	0.3325	0.6475	0.079*
C29	0.3963 (4)	0.4690 (7)	0.6492 (4)	0.0551 (19)
H29A	0.3741	0.5140	0.6665	0.066*
C30	0.4429 (3)	0.5105 (6)	0.6349 (3)	0.0372 (14)
C31	0.3631 (3)	0.7377 (6)	0.6252 (3)	0.0455 (16)
H31A	0.3640	0.7213	0.5873	0.055*
C32	0.3156 (4)	0.7850 (7)	0.6361 (4)	0.059 (2)
H32A	0.2838	0.7973	0.6058	0.071*
C33	0.3145 (4)	0.8136 (8)	0.6895 (4)	0.064 (2)
H33A	0.2820	0.8458	0.6966	0.077*
C34	0.3611 (4)	0.7957 (9)	0.7339 (4)	0.069 (3)
H34A	0.3611	0.8182	0.7712	0.083*
C35	0.4076 (4)	0.7448 (7)	0.7234 (3)	0.0533 (19)
H35A	0.4389	0.7305	0.7540	0.064*
C36	0.4087 (3)	0.7146 (6)	0.6692 (3)	0.0395 (14)
C37	0.9802 (4)	0.5462 (6)	0.2222 (4)	0.070 (2)
H37A	0.9652	0.5065	0.1864	0.084*
H37B	1.0142	0.5083	0.2432	0.084*
C38	0.9372 (4)	0.5445 (8)	0.2572 (5)	0.078 (2)
H38A	0.9243	0.4694	0.2595	0.093*
H38B	0.9551	0.5685	0.2962	0.093*
C39	0.8893 (4)	0.6122 (7)	0.2347 (5)	0.086 (2)
H39A	0.8675	0.6186	0.2637	0.103*
H39B	0.8652	0.5754	0.2014	0.103*



## supplementary materials

---

C40	0.9015 (4)	0.7225 (7)	0.2172 (5)	0.075 (2)	
H40A	0.9157	0.7670	0.2514	0.090*	
H40B	0.8664	0.7559	0.1952	0.090*	
C41	0.9441 (4)	0.7227 (7)	0.1814 (4)	0.070 (2)	
H41A	0.9268	0.6912	0.1438	0.083*	
H41B	0.9545	0.7981	0.1755	0.083*	
C42	0.9957 (4)	0.6603 (6)	0.2083 (4)	0.0654 (19)	
H42A	1.0140	0.6967	0.2448	0.078*	
C43	1.0662 (4)	0.8782 (7)	0.1958 (4)	0.063 (2)	
H43A	1.0648	0.8553	0.2327	0.075*	
C44	1.0755 (4)	0.9838 (8)	0.1865 (5)	0.074 (3)	
H44A	1.0797	1.0349	0.2164	0.089*	
C45	1.0787 (4)	1.0152 (6)	0.1339 (6)	0.073 (3)	
H45A	1.0860	1.0888	0.1276	0.088*	
C46	1.0716 (4)	0.9445 (7)	0.0901 (5)	0.075 (3)	
H46A	1.0735	0.9689	0.0536	0.090*	
C47	1.0614 (4)	0.8354 (7)	0.0989 (4)	0.060 (2)	
H47A	1.0565	0.7850	0.0687	0.072*	
C48	1.0588 (3)	0.8027 (5)	0.1521 (3)	0.0489 (18)	
C49	1.1575 (14)	0.603 (5)	0.1732 (14)	0.063 (3)	0.22 (3)
H49A	1.1472	0.5995	0.1330	0.076*	0.22 (3)
C50	1.2121 (12)	0.581 (4)	0.203 (2)	0.074 (4)	0.22 (3)
H50A	1.2391	0.5624	0.1824	0.089*	0.22 (3)
C51	1.2271 (11)	0.587 (4)	0.261 (2)	0.078 (4)	0.22 (3)
H51A	1.2644	0.5716	0.2814	0.094*	0.22 (3)
C52	1.1875 (18)	0.614 (4)	0.2909 (15)	0.090 (5)	0.22 (3)
H52A	1.1978	0.6179	0.3311	0.107*	0.22 (3)
C53	1.1329 (16)	0.636 (4)	0.2616 (16)	0.072 (4)	0.22 (3)
H53A	1.1059	0.6550	0.2818	0.086*	0.22 (3)
C54	1.1179 (10)	0.631 (5)	0.2028 (16)	0.058 (3)	0.22 (3)
C85	1.1550 (4)	0.6036 (11)	0.1920 (5)	0.063 (3)	0.78 (3)
H85A	1.1503	0.6061	0.1521	0.076*	0.78 (3)
C86	1.2076 (3)	0.5856 (10)	0.2274 (6)	0.074 (4)	0.78 (3)
H86A	1.2389	0.5757	0.2117	0.089*	0.78 (3)
C87	1.2144 (4)	0.5819 (10)	0.2858 (6)	0.078 (4)	0.78 (3)
H87A	1.2503	0.5696	0.3100	0.094*	0.78 (3)
C88	1.1686 (6)	0.5964 (10)	0.3088 (4)	0.090 (5)	0.78 (3)
H88A	1.1733	0.5939	0.3487	0.107*	0.78 (3)
C89	1.1160 (5)	0.6144 (11)	0.2734 (4)	0.072 (4)	0.78 (3)
H89A	1.0848	0.6243	0.2891	0.086*	0.78 (3)
C90	1.1092 (4)	0.6181 (11)	0.2150 (4)	0.058 (3)	0.78 (3)
C55	0.8124 (3)	0.1958 (6)	-0.1115 (3)	0.0410 (15)	
H55A	0.8203	0.1186	-0.1028	0.049*	
H55B	0.8470	0.2300	-0.1165	0.049*	
C56	0.7666 (3)	0.2062 (6)	-0.1663 (3)	0.055 (2)	
H56A	0.7800	0.1749	-0.1980	0.066*	
H56B	0.7334	0.1646	-0.1626	0.066*	
C57	0.7499 (3)	0.3227 (6)	-0.1800 (3)	0.0526 (19)	
H57A	0.7815	0.3621	-0.1888	0.063*	

H57B	0.7181	0.3253	-0.2139	0.063*	
C58	0.7333 (3)	0.3771 (8)	-0.1309 (3)	0.060 (2)	
H58A	0.7255	0.4543	-0.1399	0.072*	
H58B	0.6988	0.3436	-0.1251	0.072*	
C59	0.7791 (3)	0.3674 (6)	-0.0770 (3)	0.052 (2)	
H59A	0.7666	0.4012	-0.0454	0.062*	
H59B	0.8126	0.4067	-0.0816	0.062*	
C60	0.7944 (3)	0.2495 (6)	-0.0624 (3)	0.0432 (16)	
H60A	0.7604	0.2115	-0.0568	0.052*	
C61	0.7774 (9)	0.2483 (14)	0.0737 (10)	0.057 (3)	0.297 (12)
H61A	0.7689	0.1772	0.0597	0.069*	0.297 (12)
C62	0.7485 (9)	0.294 (2)	0.1103 (11)	0.070 (4)	0.297 (12)
H62A	0.7201	0.2534	0.1214	0.084*	0.297 (12)
C63	0.7610 (9)	0.398 (2)	0.1307 (9)	0.081 (6)	0.297 (12)
H63A	0.7412	0.4285	0.1557	0.097*	0.297 (12)
C64	0.8024 (9)	0.4563 (17)	0.1145 (9)	0.070 (4)	0.297 (12)
H64A	0.8110	0.5274	0.1285	0.084*	0.297 (12)
C65	0.8314 (8)	0.4111 (17)	0.0779 (9)	0.055 (3)	0.297 (12)
H65A	0.8597	0.4512	0.0668	0.066*	0.297 (12)
C66	0.8189 (9)	0.3071 (17)	0.0575 (9)	0.036 (2)	0.297 (12)
C79	0.7599 (3)	0.2106 (7)	0.0582 (4)	0.057 (3)	0.703 (12)
H79A	0.7536	0.1440	0.0383	0.069*	0.703 (12)
C80	0.7248 (3)	0.2428 (8)	0.0918 (4)	0.070 (4)	0.703 (12)
H80A	0.6944	0.1983	0.0950	0.084*	0.703 (12)
C81	0.7341 (4)	0.3402 (9)	0.1209 (4)	0.081 (6)	0.703 (12)
H81A	0.7100	0.3622	0.1439	0.097*	0.703 (12)
C82	0.7785 (4)	0.4053 (8)	0.1163 (4)	0.070 (4)	0.703 (12)
H82A	0.7849	0.4719	0.1361	0.084*	0.703 (12)
C83	0.8137 (3)	0.3731 (7)	0.0826 (4)	0.055 (3)	0.703 (12)
H83A	0.8441	0.4176	0.0795	0.066*	0.703 (12)
C84	0.8044 (3)	0.2757 (7)	0.0536 (3)	0.036 (2)	0.703 (12)
C67	0.9137 (3)	0.0797 (5)	0.0602 (3)	0.0364 (13)	
H67A	0.9389	0.1365	0.0750	0.044*	
C68	0.9272 (3)	-0.0280 (6)	0.0768 (3)	0.0462 (16)	
H68A	0.9617	-0.0438	0.1029	0.055*	
C69	0.8908 (4)	-0.1097 (6)	0.0555 (3)	0.0516 (19)	
H69A	0.9000	-0.1817	0.0676	0.062*	
C70	0.8409 (4)	-0.0888 (7)	0.0167 (4)	0.061 (2)	
H70A	0.8164	-0.1459	0.0009	0.073*	
C71	0.8271 (4)	0.0183 (7)	0.0011 (4)	0.058 (2)	
H71A	0.7921	0.0337	-0.0243	0.070*	
C72	0.8630 (3)	0.1016 (5)	0.0216 (3)	0.0390 (14)	

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.0498 (3)	0.0511 (4)	0.0721 (4)	-0.0034 (3)	-0.0053 (3)	0.0026 (3)
Ag2	0.0504 (3)	0.0512 (3)	0.0477 (3)	-0.0002 (3)	0.0214 (3)	0.0046 (3)

## supplementary materials

---

Ag3	0.0764 (4)	0.0337 (3)	0.0575 (4)	-0.0062 (3)	0.0067 (3)	-0.0041 (3)
Ag4	0.0405 (3)	0.0304 (3)	0.0569 (3)	0.0017 (2)	0.0022 (2)	0.0028 (2)
I1	0.0359 (2)	0.0399 (2)	0.0495 (3)	0.00681 (18)	0.01294 (19)	0.00699 (19)
I2	0.0532 (3)	0.0412 (3)	0.0620 (3)	0.0034 (2)	0.0033 (2)	-0.0064 (2)
I3	0.0619 (3)	0.0273 (2)	0.0531 (3)	0.0066 (2)	-0.0005 (2)	-0.00548 (19)
I4	0.0363 (2)	0.02788 (19)	0.0439 (2)	0.00317 (16)	0.00288 (17)	0.00464 (17)
P1	0.0396 (9)	0.0375 (9)	0.0478 (10)	-0.0014 (8)	0.0057 (8)	0.0066 (8)
P2	0.0306 (8)	0.0367 (9)	0.0320 (8)	0.0008 (7)	0.0063 (6)	0.0012 (7)
P3	0.0752 (15)	0.0266 (9)	0.0516 (11)	-0.0001 (9)	0.0101 (10)	-0.0013 (8)
P4	0.0325 (8)	0.0401 (9)	0.0380 (8)	0.0070 (7)	0.0069 (7)	0.0079 (7)
C1	0.057 (5)	0.041 (4)	0.054 (4)	0.008 (3)	0.015 (4)	0.011 (3)
C2	0.050 (5)	0.038 (4)	0.082 (6)	-0.007 (3)	0.023 (4)	0.005 (4)
C3	0.055 (5)	0.048 (4)	0.067 (5)	-0.003 (4)	0.022 (4)	-0.005 (4)
C4	0.067 (6)	0.053 (5)	0.075 (6)	0.014 (4)	0.027 (5)	-0.003 (5)
C5	0.077 (6)	0.034 (4)	0.057 (5)	0.005 (4)	0.021 (4)	0.006 (3)
C6	0.053 (4)	0.041 (4)	0.048 (4)	0.007 (3)	0.017 (3)	0.004 (3)
C7	0.036 (6)	0.059 (8)	0.052 (5)	0.021 (5)	0.009 (4)	0.002 (5)
C8	0.064 (5)	0.084 (10)	0.045 (4)	0.015 (5)	0.008 (4)	0.002 (6)
C9	0.104 (11)	0.102 (8)	0.044 (6)	0.004 (8)	0.011 (6)	0.022 (5)
C10	0.108 (11)	0.097 (12)	0.060 (7)	-0.020 (9)	0.005 (8)	0.039 (8)
C11	0.077 (7)	0.069 (11)	0.070 (6)	-0.008 (7)	0.013 (5)	0.030 (8)
C12	0.039 (4)	0.049 (4)	0.057 (4)	0.008 (3)	0.015 (3)	0.014 (3)
C73	0.036 (6)	0.059 (8)	0.052 (5)	0.021 (5)	0.009 (4)	0.002 (5)
C74	0.064 (5)	0.084 (10)	0.045 (4)	0.015 (5)	0.008 (4)	0.002 (6)
C75	0.104 (11)	0.102 (8)	0.044 (6)	0.004 (8)	0.011 (6)	0.022 (5)
C76	0.108 (11)	0.097 (12)	0.060 (7)	-0.020 (9)	0.005 (8)	0.039 (8)
C77	0.077 (7)	0.069 (11)	0.070 (6)	-0.008 (7)	0.013 (5)	0.030 (8)
C78	0.039 (4)	0.049 (4)	0.057 (4)	0.008 (3)	0.015 (3)	0.014 (3)
C13	0.052 (5)	0.050 (5)	0.059 (5)	0.011 (4)	0.001 (4)	0.011 (4)
C14	0.058 (5)	0.058 (5)	0.049 (4)	0.002 (4)	0.005 (4)	0.001 (4)
C15	0.057 (5)	0.047 (4)	0.067 (5)	0.008 (4)	0.029 (4)	0.001 (4)
C16	0.064 (5)	0.060 (5)	0.053 (5)	0.025 (4)	0.021 (4)	0.013 (4)
C17	0.057 (5)	0.068 (6)	0.051 (4)	0.018 (4)	0.017 (4)	-0.003 (4)
C18	0.039 (3)	0.039 (4)	0.039 (3)	0.000 (3)	0.008 (3)	0.007 (3)
C19	0.040 (4)	0.038 (4)	0.068 (5)	-0.004 (3)	-0.001 (3)	-0.003 (4)
C20	0.056 (5)	0.049 (5)	0.055 (5)	-0.006 (4)	-0.006 (4)	-0.016 (4)
C21	0.046 (4)	0.069 (6)	0.050 (5)	0.006 (4)	0.001 (3)	-0.006 (4)
C22	0.061 (5)	0.054 (5)	0.051 (5)	0.018 (4)	-0.007 (4)	-0.002 (4)
C23	0.052 (5)	0.053 (5)	0.062 (5)	0.015 (4)	0.002 (4)	-0.007 (4)
C24	0.033 (3)	0.035 (3)	0.040 (3)	0.001 (3)	0.000 (3)	-0.007 (3)
C25	0.054 (5)	0.060 (5)	0.055 (5)	-0.020 (4)	0.013 (4)	-0.020 (4)
C26	0.071 (6)	0.061 (5)	0.065 (5)	-0.007 (5)	0.021 (4)	-0.023 (5)
C27	0.085 (7)	0.046 (5)	0.050 (4)	-0.022 (4)	0.008 (4)	-0.013 (4)
C28	0.059 (5)	0.057 (5)	0.079 (6)	-0.021 (4)	0.013 (5)	-0.002 (5)
C29	0.054 (5)	0.051 (4)	0.061 (5)	-0.006 (4)	0.015 (4)	0.001 (4)
C30	0.035 (3)	0.039 (3)	0.035 (3)	-0.006 (3)	0.003 (3)	-0.001 (3)
C31	0.042 (4)	0.048 (4)	0.048 (4)	0.004 (3)	0.014 (3)	-0.002 (3)
C32	0.046 (5)	0.060 (5)	0.068 (5)	0.010 (4)	0.005 (4)	0.003 (4)
C33	0.046 (5)	0.064 (6)	0.086 (6)	0.011 (4)	0.023 (4)	-0.014 (5)

## supplementary materials

C34	0.071 (6)	0.079 (7)	0.065 (6)	0.007 (5)	0.030 (5)	-0.020 (5)
C35	0.053 (4)	0.055 (5)	0.050 (4)	0.003 (4)	0.008 (3)	-0.007 (4)
C36	0.035 (3)	0.039 (3)	0.047 (4)	0.004 (3)	0.015 (3)	0.001 (3)
C37	0.099 (5)	0.040 (3)	0.079 (5)	0.006 (4)	0.035 (4)	0.010 (4)
C38	0.103 (6)	0.054 (4)	0.086 (5)	0.006 (4)	0.042 (4)	0.012 (4)
C39	0.097 (5)	0.068 (5)	0.100 (6)	0.006 (4)	0.039 (5)	0.017 (4)
C40	0.080 (5)	0.058 (4)	0.085 (5)	0.012 (4)	0.017 (4)	0.010 (4)
C41	0.077 (5)	0.050 (4)	0.076 (5)	-0.001 (3)	0.007 (4)	0.022 (4)
C42	0.087 (5)	0.037 (3)	0.074 (5)	0.007 (3)	0.024 (4)	0.008 (3)
C43	0.073 (6)	0.039 (4)	0.071 (6)	0.001 (4)	0.007 (5)	-0.012 (4)
C44	0.057 (6)	0.044 (5)	0.108 (8)	-0.004 (4)	-0.007 (5)	-0.021 (5)
C45	0.042 (5)	0.028 (4)	0.161 (11)	-0.002 (3)	0.046 (6)	-0.009 (5)
C46	0.089 (7)	0.031 (4)	0.121 (9)	0.003 (4)	0.057 (7)	0.015 (5)
C47	0.076 (6)	0.034 (4)	0.076 (6)	0.003 (4)	0.033 (5)	0.003 (4)
C48	0.060 (5)	0.023 (3)	0.060 (5)	-0.003 (3)	0.008 (4)	-0.003 (3)
C49	0.083 (6)	0.056 (6)	0.047 (6)	-0.008 (5)	0.008 (5)	0.004 (6)
C50	0.083 (6)	0.066 (6)	0.067 (8)	0.009 (6)	0.007 (6)	-0.004 (7)
C51	0.089 (7)	0.065 (6)	0.067 (8)	0.024 (7)	-0.007 (6)	0.004 (8)
C52	0.111 (9)	0.098 (9)	0.045 (6)	0.050 (9)	-0.007 (5)	0.006 (7)
C53	0.085 (7)	0.075 (9)	0.052 (6)	0.010 (7)	0.009 (5)	0.001 (6)
C54	0.083 (6)	0.034 (5)	0.048 (6)	0.018 (5)	0.000 (4)	0.003 (5)
C85	0.083 (6)	0.056 (6)	0.047 (6)	-0.008 (5)	0.008 (5)	0.004 (6)
C86	0.083 (6)	0.066 (6)	0.067 (8)	0.009 (6)	0.007 (6)	-0.004 (7)
C87	0.089 (7)	0.065 (6)	0.067 (8)	0.024 (7)	-0.007 (6)	0.004 (8)
C88	0.111 (9)	0.098 (9)	0.045 (6)	0.050 (9)	-0.007 (5)	0.006 (7)
C89	0.085 (7)	0.075 (9)	0.052 (6)	0.010 (7)	0.009 (5)	0.001 (6)
C90	0.083 (6)	0.034 (5)	0.048 (6)	0.018 (5)	0.000 (4)	0.003 (5)
C55	0.033 (3)	0.042 (4)	0.045 (4)	0.000 (3)	0.005 (3)	0.002 (3)
C56	0.053 (4)	0.067 (5)	0.042 (4)	-0.017 (4)	0.006 (3)	0.002 (4)
C57	0.049 (4)	0.067 (5)	0.041 (4)	0.000 (4)	0.010 (3)	0.019 (4)
C58	0.048 (4)	0.081 (6)	0.052 (5)	0.021 (4)	0.013 (4)	0.020 (4)
C59	0.046 (4)	0.065 (5)	0.046 (4)	0.018 (4)	0.014 (3)	0.020 (4)
C60	0.028 (3)	0.053 (4)	0.043 (4)	0.006 (3)	-0.001 (3)	0.013 (3)
C61	0.030 (6)	0.084 (10)	0.058 (7)	-0.003 (6)	0.011 (5)	0.016 (7)
C62	0.035 (7)	0.108 (13)	0.070 (8)	0.002 (6)	0.019 (6)	0.029 (8)
C63	0.059 (9)	0.142 (18)	0.046 (6)	0.025 (9)	0.017 (7)	0.016 (9)
C64	0.049 (8)	0.104 (13)	0.061 (7)	0.012 (7)	0.021 (6)	-0.001 (8)
C65	0.050 (7)	0.063 (9)	0.052 (6)	0.005 (6)	0.015 (5)	0.010 (6)
C66	0.023 (5)	0.049 (7)	0.034 (4)	-0.001 (4)	0.003 (4)	0.016 (4)
C79	0.030 (6)	0.084 (10)	0.058 (7)	-0.003 (6)	0.011 (5)	0.016 (7)
C80	0.035 (7)	0.108 (13)	0.070 (8)	0.002 (6)	0.019 (6)	0.029 (8)
C81	0.059 (9)	0.142 (18)	0.046 (6)	0.025 (9)	0.017 (7)	0.016 (9)
C82	0.049 (8)	0.104 (13)	0.061 (7)	0.012 (7)	0.021 (6)	-0.001 (8)
C83	0.050 (7)	0.063 (9)	0.052 (6)	0.005 (6)	0.015 (5)	0.010 (6)
C84	0.023 (5)	0.049 (7)	0.034 (4)	-0.001 (4)	0.003 (4)	0.016 (4)
C67	0.036 (3)	0.032 (3)	0.039 (3)	0.001 (3)	0.006 (3)	0.003 (3)
C68	0.046 (4)	0.035 (3)	0.053 (4)	0.000 (3)	0.004 (3)	0.006 (3)
C69	0.067 (5)	0.035 (4)	0.049 (4)	-0.008 (4)	0.007 (4)	0.009 (3)
C70	0.077 (6)	0.046 (5)	0.056 (5)	-0.029 (4)	0.010 (4)	0.010 (4)

## supplementary materials

---

C71	0.048 (4)	0.062 (5)	0.058 (5)	-0.017 (4)	-0.003 (4)	0.017 (4)
C72	0.035 (3)	0.033 (3)	0.047 (4)	0.002 (3)	0.006 (3)	0.002 (3)

### *Geometric parameters (Å, °)*

Ag1—P1	2.450 (2)	C29—H29A	0.9500
Ag1—I2 <sup>i</sup>	2.8129 (13)	C31—C36	1.382 (10)
Ag1—I1	2.9334 (14)	C31—C32	1.392 (11)
Ag1—I2	2.9808 (13)	C31—H31A	0.9500
Ag2—P2	2.4503 (19)	C32—C33	1.353 (12)
Ag2—I1	2.8163 (11)	C32—H32A	0.9500
Ag2—I2	2.9199 (14)	C33—C34	1.391 (13)
Ag2—I1 <sup>i</sup>	2.9595 (11)	C33—H33A	0.9500
Ag3—P3	2.444 (2)	C34—C35	1.387 (12)
Ag3—I4	2.8700 (13)	C34—H34A	0.9500
Ag3—I3	2.8846 (12)	C35—C36	1.379 (10)
Ag3—I3 <sup>ii</sup>	2.9355 (12)	C35—H35A	0.9500
Ag4—P4	2.450 (2)	C37—C38	1.515 (10)
Ag4—I4	2.9029 (10)	C37—C42	1.526 (9)
Ag4—I4 <sup>ii</sup>	2.9175 (12)	C37—H37A	0.9900
Ag4—I3	2.9176 (13)	C37—H37B	0.9900
I1—Ag2 <sup>i</sup>	2.9593 (11)	C38—C39	1.445 (10)
I2—Ag1 <sup>i</sup>	2.8129 (13)	C38—H38A	0.9900
I3—Ag3 <sup>ii</sup>	2.9355 (12)	C38—H38B	0.9900
I4—Ag4 <sup>ii</sup>	2.9176 (12)	C39—C40	1.486 (10)
P1—C18	1.831 (7)	C39—H39A	0.9900
P1—C78	1.831 (14)	C39—H39B	0.9900
P1—C12	1.858 (8)	C40—C41	1.520 (10)
P1—C6	1.865 (8)	C40—H40A	0.9900
P2—C30	1.825 (7)	C40—H40B	0.9900
P2—C36	1.838 (7)	C41—C42	1.499 (10)
P2—C24	1.839 (7)	C41—H41A	0.9900
P3—C42	1.822 (9)	C41—H41B	0.9900
P3—C90	1.834 (6)	C42—H42A	1.0000
P3—C48	1.834 (7)	C43—C44	1.358 (13)
P3—C54	1.850 (16)	C43—C48	1.396 (11)
P4—C66	1.818 (12)	C43—H43A	0.9500
P4—C72	1.821 (7)	C44—C45	1.359 (16)
P4—C60	1.843 (7)	C44—H44A	0.9500
P4—C84	1.854 (5)	C45—C46	1.358 (15)
C1—C6	1.495 (11)	C45—H45A	0.9500
C1—C2	1.517 (11)	C46—C47	1.403 (11)
C1—H1A	0.9900	C46—H46A	0.9500
C1—H1B	0.9900	C47—C48	1.371 (12)
C2—C3	1.521 (11)	C47—H47A	0.9500
C2—H2A	0.9900	C49—C50	1.3900
C2—H2B	0.9900	C49—C54	1.3900

## supplementary materials

C3—C4	1.496 (13)	C49—H49A	0.9500
C3—H3A	0.9900	C50—C51	1.3705
C3—H3B	0.9900	C50—H50A	0.9500
C4—C5	1.549 (12)	C51—C52	1.3900
C4—H4A	0.9900	C51—H51A	0.9500
C4—H4B	0.9900	C52—C53	1.3900
C5—C6	1.525 (10)	C52—H52A	0.9500
C5—H5A	0.9900	C53—C54	1.3900
C5—H5B	0.9900	C53—H53A	0.9500
C6—H6A	1.0000	C85—C86	1.3900
C7—C8	1.3900	C85—C90	1.3900
C7—C12	1.3900	C85—H85A	0.9500
C7—H7A	0.9500	C86—C87	1.3900
C8—C9	1.3900	C86—H86A	0.9500
C8—H8A	0.9500	C87—C88	1.3900
C9—C10	1.3900	C87—H87A	0.9500
C9—H9A	0.9500	C88—C89	1.3900
C10—C11	1.3900	C88—H88A	0.9500
C10—H10A	0.9500	C89—C90	1.3900
C11—C12	1.3900	C89—H89A	0.9500
C11—H11A	0.9500	C55—C60	1.526 (8)
C73—C74	1.3900	C55—C56	1.529 (8)
C73—C78	1.3900	C55—H55A	0.9900
C73—H73A	0.9500	C55—H55B	0.9900
C74—C75	1.3900	C56—C57	1.516 (9)
C74—H74A	0.9500	C56—H56A	0.9900
C75—C76	1.3900	C56—H56B	0.9900
C75—H75A	0.9500	C57—C58	1.513 (9)
C76—C77	1.3900	C57—H57A	0.9900
C76—H76A	0.9500	C57—H57B	0.9900
C77—C78	1.3900	C58—C59	1.512 (9)
C77—H77A	0.9500	C58—H58A	0.9900
C13—C14	1.378 (12)	C58—H58B	0.9900
C13—C18	1.387 (11)	C59—C60	1.530 (9)
C13—H13A	0.9500	C59—H59A	0.9900
C14—C15	1.374 (12)	C59—H59B	0.9900
C14—H14A	0.9500	C60—H60A	1.0000
C15—C16	1.370 (12)	C61—C62	1.3900
C15—H15A	0.9500	C61—C66	1.3900
C16—C17	1.392 (12)	C61—H61A	0.9500
C16—H16A	0.9500	C62—C63	1.3900
C17—C18	1.389 (11)	C62—H62A	0.9500
C17—H17A	0.9500	C63—C64	1.3900
C19—C24	1.530 (10)	C63—H63A	0.9500
C19—C20	1.540 (11)	C64—C65	1.3900
C19—H19A	0.9900	C64—H64A	0.9500
C19—H19B	0.9900	C65—C66	1.3900
C20—C21	1.500 (12)	C65—H65A	0.9500
C20—H20A	0.9900	C79—C80	1.3900

## supplementary materials

---

C20—H20B	0.9900	C79—C84	1.3900
C21—C22	1.480 (13)	C79—H79A	0.9500
C21—H21A	0.9900	C80—C81	1.3900
C21—H21B	0.9900	C80—H80A	0.9500
C22—C23	1.536 (11)	C81—C82	1.3900
C22—H22A	0.9900	C81—H81A	0.9500
C22—H22B	0.9900	C82—C83	1.3900
C23—C24	1.500 (10)	C82—H82A	0.9500
C23—H23A	0.9900	C83—C84	1.3900
C23—H23B	0.9900	C83—H83A	0.9500
C24—H24A	1.0000	C67—C72	1.395 (9)
C25—C30	1.367 (11)	C67—C68	1.412 (10)
C25—C26	1.393 (13)	C67—H67A	0.9500
C25—H25A	0.9500	C68—C69	1.370 (10)
C26—C27	1.355 (13)	C68—H68A	0.9500
C26—H26A	0.9500	C69—C70	1.382 (12)
C27—C28	1.378 (13)	C69—H69A	0.9500
C27—H27A	0.9500	C70—C71	1.400 (12)
C28—C29	1.403 (12)	C70—H70A	0.9500
C28—H28A	0.9500	C71—C72	1.375 (10)
C29—C30	1.381 (10)	C71—H71A	0.9500
P1—Ag1—I2 <sup>i</sup>	122.00 (5)	C29—C28—H28A	119.8
P1—Ag1—I1	113.51 (5)	C30—C29—C28	120.2 (8)
I2 <sup>i</sup> —Ag1—I1	103.73 (3)	C30—C29—H29A	119.9
P1—Ag1—I2	109.75 (6)	C28—C29—H29A	119.9
I2 <sup>i</sup> —Ag1—I2	102.17 (4)	C25—C30—C29	117.8 (7)
I1—Ag1—I2	103.71 (3)	C25—C30—P2	117.9 (5)
P2—Ag2—I1	124.64 (5)	C29—C30—P2	124.3 (6)
P2—Ag2—I2	109.52 (5)	C36—C31—C32	120.4 (7)
I1—Ag2—I2	108.35 (2)	C36—C31—H31A	119.8
P2—Ag2—I1 <sup>i</sup>	110.27 (5)	C32—C31—H31A	119.8
I1—Ag2—I1 <sup>i</sup>	100.68 (3)	C33—C32—C31	120.6 (8)
I2—Ag2—I1 <sup>i</sup>	100.50 (2)	C33—C32—H32A	119.7
P3—Ag3—I4	111.91 (6)	C31—C32—H32A	119.7
P3—Ag3—I3	118.03 (7)	C32—C33—C34	119.8 (8)
I4—Ag3—I3	104.40 (2)	C32—C33—H33A	120.1
P3—Ag3—I3 <sup>ii</sup>	116.12 (7)	C34—C33—H33A	120.1
I4—Ag3—I3 <sup>ii</sup>	102.95 (3)	C35—C34—C33	119.7 (8)
I3—Ag3—I3 <sup>ii</sup>	101.63 (4)	C35—C34—H34A	120.2
P4—Ag4—I4	116.69 (5)	C33—C34—H34A	120.2
P4—Ag4—I4 <sup>ii</sup>	114.43 (5)	C36—C35—C34	120.7 (8)
I4—Ag4—I4 <sup>ii</sup>	105.99 (3)	C36—C35—H35A	119.6
P4—Ag4—I3	113.15 (5)	C34—C35—H35A	119.6
I4—Ag4—I3	102.74 (2)	C35—C36—C31	118.7 (7)
I4 <sup>ii</sup> —Ag4—I3	102.23 (2)	C35—C36—P2	125.0 (6)
Ag2—I1—Ag1	74.23 (2)	C31—C36—P2	116.2 (5)

Ag2—I1—Ag2 <sup>i</sup>	76.55 (3)	C38—C37—C42	112.7 (7)
Ag1—I1—Ag2 <sup>i</sup>	74.39 (2)	C38—C37—H37A	109.0
Ag1 <sup>i</sup> —I2—Ag2	76.81 (2)	C42—C37—H37A	109.0
Ag1 <sup>i</sup> —I2—Ag1	75.36 (4)	C38—C37—H37B	109.0
Ag2—I2—Ag1	72.05 (2)	C42—C37—H37B	109.0
Ag3—I3—Ag4	74.43 (2)	H37A—C37—H37B	107.8
Ag3—I3—Ag3 <sup>ii</sup>	76.51 (4)	C39—C38—C37	113.6 (7)
Ag4—I3—Ag3 <sup>ii</sup>	74.78 (2)	C39—C38—H38A	108.8
Ag3—I4—Ag4	74.87 (2)	C37—C38—H38A	108.9
Ag3—I4—Ag4 <sup>ii</sup>	75.78 (2)	C39—C38—H38B	108.9
Ag4—I4—Ag4 <sup>ii</sup>	72.57 (3)	C37—C38—H38B	108.9
C18—P1—C78	105.6 (11)	H38A—C38—H38B	107.7
C18—P1—C12	105.4 (5)	C38—C39—C40	116.1 (7)
C18—P1—C6	102.9 (3)	C38—C39—H39A	108.3
C78—P1—C6	97.5 (11)	C40—C39—H39A	108.3
C12—P1—C6	103.0 (6)	C38—C39—H39B	108.3
C18—P1—Ag1	114.3 (2)	C40—C39—H39B	108.3
C78—P1—Ag1	117.5 (11)	H39A—C39—H39B	107.4
C12—P1—Ag1	113.0 (5)	C39—C40—C41	112.5 (7)
C6—P1—Ag1	116.7 (3)	C39—C40—H40A	109.1
C30—P2—C36	102.5 (3)	C41—C40—H40A	109.1
C30—P2—C24	102.5 (3)	C39—C40—H40B	109.1
C36—P2—C24	103.5 (3)	C41—C40—H40B	109.1
C30—P2—Ag2	116.5 (2)	H40A—C40—H40B	107.8
C36—P2—Ag2	110.7 (2)	C42—C41—C40	112.7 (7)
C24—P2—Ag2	119.1 (2)	C42—C41—H41A	109.1
C42—P3—C90	100.8 (5)	C40—C41—H41A	109.1
C42—P3—C48	105.4 (4)	C42—C41—H41B	109.1
C90—P3—C48	102.7 (5)	C40—C41—H41B	109.1
C42—P3—C54	113.7 (13)	H41A—C41—H41B	107.8
C48—P3—C54	94.5 (18)	C41—C42—C37	110.0 (7)
C42—P3—Ag3	116.7 (3)	C41—C42—P3	111.4 (6)
C90—P3—Ag3	115.8 (4)	C37—C42—P3	111.9 (6)
C48—P3—Ag3	113.6 (3)	C41—C42—H42A	107.8
C54—P3—Ag3	110.6 (16)	C37—C42—H42A	107.8
C66—P4—C72	110.2 (8)	P3—C42—H42A	107.8
C66—P4—C60	105.8 (8)	C44—C43—C48	121.0 (10)
C72—P4—C60	107.5 (3)	C44—C43—H43A	119.5
C72—P4—C84	99.9 (4)	C48—C43—H43A	119.5
C60—P4—C84	98.1 (4)	C43—C44—C45	119.0 (10)
C66—P4—Ag4	104.5 (6)	C43—C44—H44A	120.5
C72—P4—Ag4	115.2 (2)	C45—C44—H44A	120.5
C60—P4—Ag4	113.3 (2)	C46—C45—C44	121.9 (8)
C84—P4—Ag4	120.7 (3)	C46—C45—H45A	119.1
C6—C1—C2	110.7 (7)	C44—C45—H45A	119.1
C6—C1—H1A	109.5	C45—C46—C47	119.8 (10)
C2—C1—H1A	109.5	C45—C46—H46A	120.1



## supplementary materials

---

C6—C1—H1B	109.5	C47—C46—H46A	120.1
C2—C1—H1B	109.5	C48—C47—C46	118.7 (9)
H1A—C1—H1B	108.1	C48—C47—H47A	120.6
C1—C2—C3	111.7 (7)	C46—C47—H47A	120.6
C1—C2—H2A	109.3	C47—C48—C43	119.6 (7)
C3—C2—H2A	109.3	C47—C48—P3	118.8 (6)
C1—C2—H2B	109.3	C43—C48—P3	121.6 (7)
C3—C2—H2B	109.3	C50—C49—C54	120.0
H2A—C2—H2B	107.9	C50—C49—H49A	120.0
C4—C3—C2	111.3 (7)	C54—C49—H49A	120.0
C4—C3—H3A	109.4	C51—C50—C49	120.0
C2—C3—H3A	109.4	C51—C50—H50A	120.0
C4—C3—H3B	109.4	C49—C50—H50A	120.0
C2—C3—H3B	109.4	C52—C51—C50	120.0
H3A—C3—H3B	108.0	C52—C51—H51A	120.0
C3—C4—C5	111.2 (7)	C50—C51—H51A	120.0
C3—C4—H4A	109.4	C51—C52—C53	120.0
C5—C4—H4A	109.4	C51—C52—H52A	120.0
C3—C4—H4B	109.4	C53—C52—H52A	120.0
C5—C4—H4B	109.4	C54—C53—C52	120.0
H4A—C4—H4B	108.0	C54—C53—H53A	120.0
C6—C5—C4	110.4 (7)	C52—C53—H53A	120.0
C6—C5—H5A	109.6	C53—C54—C49	120.0
C4—C5—H5A	109.6	C53—C54—P3	120 (2)
C6—C5—H5B	109.6	C49—C54—P3	120 (2)
C4—C5—H5B	109.6	C86—C85—C90	120.0
H5A—C5—H5B	108.1	C86—C85—H85A	120.0
C1—C6—C5	110.6 (7)	C90—C85—H85A	120.0
C1—C6—P1	114.0 (6)	C85—C86—C87	120.0
C5—C6—P1	110.2 (5)	C85—C86—H86A	120.0
C1—C6—H6A	107.2	C87—C86—H86A	120.0
C5—C6—H6A	107.2	C88—C87—C86	120.0
P1—C6—H6A	107.2	C88—C87—H87A	120.0
C8—C7—C12	120.0	C86—C87—H87A	120.0
C8—C7—H7A	120.0	C87—C88—C89	120.0
C12—C7—H7A	120.0	C87—C88—H88A	120.0
C9—C8—C7	120.0	C89—C88—H88A	120.0
C9—C8—H8A	120.0	C90—C89—C88	120.0
C7—C8—H8A	120.0	C90—C89—H89A	120.0
C8—C9—C10	120.0	C88—C89—H89A	120.0
C8—C9—H9A	120.0	C89—C90—C85	120.0
C10—C9—H9A	120.0	C89—C90—P3	125.0 (6)
C11—C10—C9	120.0	C85—C90—P3	114.4 (5)
C11—C10—H10A	120.0	C60—C55—C56	110.5 (5)
C9—C10—H10A	120.0	C60—C55—H55A	109.5
C12—C11—C10	120.0	C56—C55—H55A	109.5
C12—C11—H11A	120.0	C60—C55—H55B	109.5
C10—C11—H11A	120.0	C56—C55—H55B	109.5
C11—C12—C7	120.0	H55A—C55—H55B	108.1

## supplementary materials

C11—C12—P1	119.3 (9)	C57—C56—C55	112.0 (6)
C7—C12—P1	119.5 (10)	C57—C56—H56A	109.2
C74—C73—C78	120.0	C55—C56—H56A	109.2
C74—C73—H73A	120.0	C57—C56—H56B	109.2
C78—C73—H73A	120.0	C55—C56—H56B	109.2
C73—C74—C75	120.0	H56A—C56—H56B	107.9
C73—C74—H74A	120.0	C58—C57—C56	111.4 (6)
C75—C74—H74A	120.0	C58—C57—H57A	109.4
C74—C75—C76	120.0	C56—C57—H57A	109.4
C74—C75—H75A	120.0	C58—C57—H57B	109.4
C76—C75—H75A	120.0	C56—C57—H57B	109.4
C77—C76—C75	120.0	H57A—C57—H57B	108.0
C77—C76—H76A	120.0	C59—C58—C57	111.1 (6)
C75—C76—H76A	120.0	C59—C58—H58A	109.4
C76—C77—C78	120.0	C57—C58—H58A	109.4
C76—C77—H77A	120.0	C59—C58—H58B	109.4
C78—C77—H77A	120.0	C57—C58—H58B	109.4
C77—C78—C73	120.0	H58A—C58—H58B	108.0
C77—C78—P1	106 (2)	C58—C59—C60	111.5 (7)
C73—C78—P1	134 (2)	C58—C59—H59A	109.3
C14—C13—C18	121.0 (8)	C60—C59—H59A	109.3
C14—C13—H13A	119.5	C58—C59—H59B	109.3
C18—C13—H13A	119.5	C60—C59—H59B	109.3
C15—C14—C13	120.1 (8)	H59A—C59—H59B	108.0
C15—C14—H14A	119.9	C55—C60—C59	109.8 (6)
C13—C14—H14A	119.9	C55—C60—P4	112.5 (4)
C16—C15—C14	119.5 (8)	C59—C60—P4	109.3 (5)
C16—C15—H15A	120.3	C55—C60—H60A	108.4
C14—C15—H15A	120.3	C59—C60—H60A	108.4
C15—C16—C17	121.1 (8)	P4—C60—H60A	108.4
C15—C16—H16A	119.5	C62—C61—C66	120.0
C17—C16—H16A	119.5	C62—C61—H61A	120.0
C18—C17—C16	119.5 (8)	C66—C61—H61A	120.0
C18—C17—H17A	120.3	C61—C62—C63	120.0
C16—C17—H17A	120.3	C61—C62—H62A	120.0
C13—C18—C17	118.7 (7)	C63—C62—H62A	120.0
C13—C18—P1	124.7 (6)	C62—C63—C64	120.0
C17—C18—P1	116.3 (6)	C62—C63—H63A	120.0
C24—C19—C20	111.2 (6)	C64—C63—H63A	120.0
C24—C19—H19A	109.4	C65—C64—C63	120.0
C20—C19—H19A	109.4	C65—C64—H64A	120.0
C24—C19—H19B	109.4	C63—C64—H64A	120.0
C20—C19—H19B	109.4	C66—C65—C64	120.0
H19A—C19—H19B	108.0	C66—C65—H65A	120.0
C21—C20—C19	111.7 (7)	C64—C65—H65A	120.0
C21—C20—H20A	109.3	C65—C66—C61	120.0
C19—C20—H20A	109.3	C65—C66—P4	124.3 (11)
C21—C20—H20B	109.3	C61—C66—P4	115.4 (11)
C19—C20—H20B	109.3	C80—C79—C84	120.0

## supplementary materials

---

H20A—C20—H20B	107.9	C80—C79—H79A	120.0
C22—C21—C20	113.1 (7)	C84—C79—H79A	120.0
C22—C21—H21A	109.0	C81—C80—C79	120.0
C20—C21—H21A	109.0	C81—C80—H80A	120.0
C22—C21—H21B	109.0	C79—C80—H80A	120.0
C20—C21—H21B	109.0	C80—C81—C82	120.0
H21A—C21—H21B	107.8	C80—C81—H81A	120.0
C21—C22—C23	111.9 (7)	C82—C81—H81A	120.0
C21—C22—H22A	109.2	C83—C82—C81	120.0
C23—C22—H22A	109.2	C83—C82—H82A	120.0
C21—C22—H22B	109.2	C81—C82—H82A	120.0
C23—C22—H22B	109.2	C84—C83—C82	120.0
H22A—C22—H22B	107.9	C84—C83—H83A	120.0
C24—C23—C22	110.9 (7)	C82—C83—H83A	120.0
C24—C23—H23A	109.5	C83—C84—C79	120.0
C22—C23—H23A	109.5	C83—C84—P4	117.8 (4)
C24—C23—H23B	109.5	C79—C84—P4	122.0 (4)
C22—C23—H23B	109.5	C72—C67—C68	119.1 (6)
H23A—C23—H23B	108.0	C72—C67—H67A	120.4
C23—C24—C19	109.7 (6)	C68—C67—H67A	120.4
C23—C24—P2	114.2 (5)	C69—C68—C67	120.3 (7)
C19—C24—P2	111.3 (5)	C69—C68—H68A	119.8
C23—C24—H24A	107.1	C67—C68—H68A	119.8
C19—C24—H24A	107.1	C68—C69—C70	120.8 (7)
P2—C24—H24A	107.1	C68—C69—H69A	119.6
C30—C25—C26	122.3 (8)	C70—C69—H69A	119.6
C30—C25—H25A	118.8	C69—C70—C71	118.8 (8)
C26—C25—H25A	118.8	C69—C70—H70A	120.6
C27—C26—C25	119.5 (8)	C71—C70—H70A	120.6
C27—C26—H26A	120.3	C72—C71—C70	121.4 (8)
C25—C26—H26A	120.3	C72—C71—H71A	119.3
C26—C27—C28	119.7 (8)	C70—C71—H71A	119.3
C26—C27—H27A	120.2	C71—C72—C67	119.5 (7)
C28—C27—H27A	120.2	C71—C72—P4	124.9 (6)
C27—C28—C29	120.3 (8)	C67—C72—P4	115.6 (5)
C27—C28—H28A	119.8		

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

Fig. 1

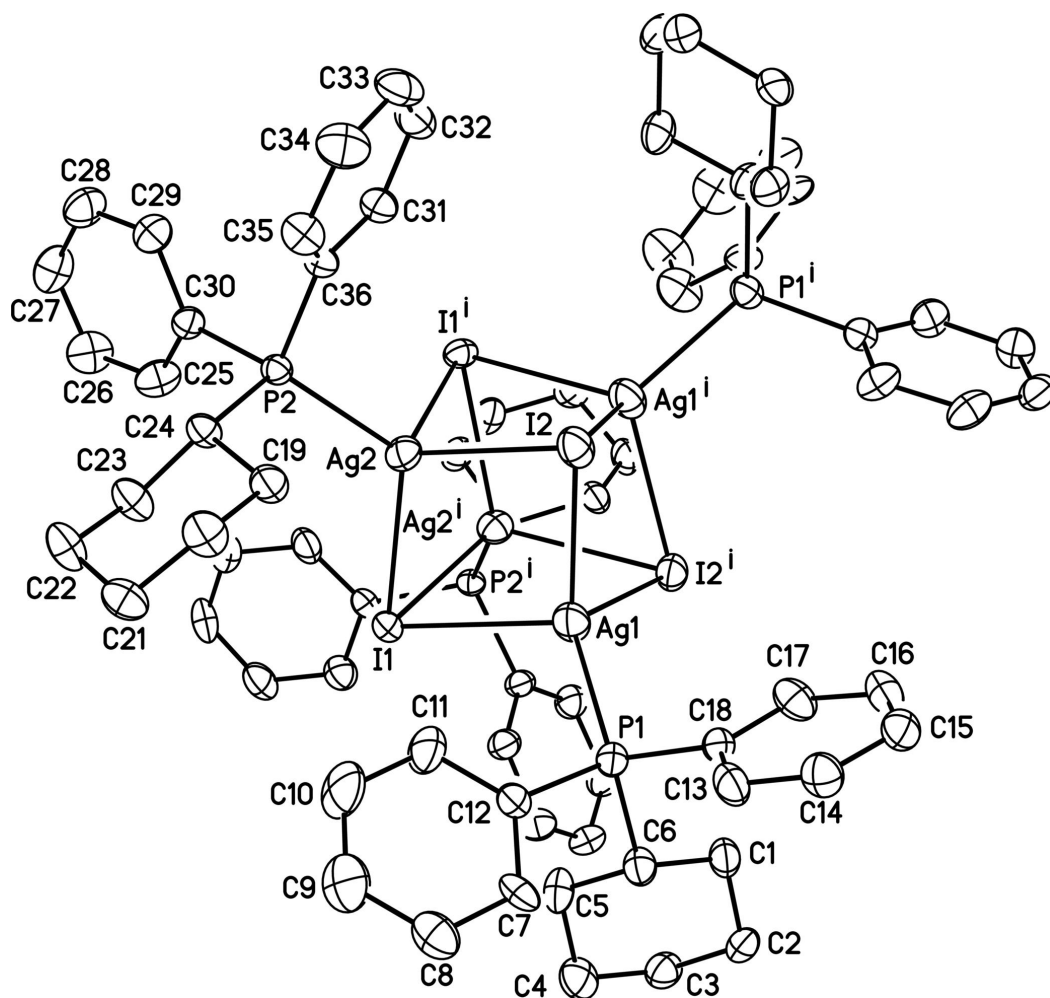


Fig. 2

