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μ_3-Iodido-tri-μ_3-sulfido-tris[(triphenylphosphine)silver(I)][thioxotungsten(VI)] dichloromethane 0.45-solvate

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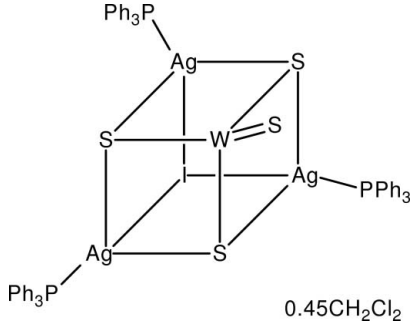
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.028; wR factor = 0.068; data-to-parameter ratio = 20.3.

In the title complex, $[WAg_3IS_4(C_{18}H_{15}P)_3]\cdot 0.45CH_2Cl_2$, the W atom has almost regular tetrahedral coordination geometry, with one terminal and three triply bridging S atoms; the Ag atoms have tetrahedral coordination geometry distorted by expanded P—Ag—S and contracted S—Ag—S angles, the fourth site being occupied by a triply bridging I atom. The bridging S and I atoms, together with the W and three Ag atoms, form a pseudo-cubane core with small angles at the non-metal vertices, resulting in short W···Ag distances. The dichloromethane solvent molecule is disordered over two inversion-related sites with common Cl-atom sites and with a refined occupancy factor of 0.449 (4) for each site.

Related literature

For similar structures, see: Jin *et al.* (1999, 2000); Sakane *et al.* (1996); Wang *et al.* (2003); Lang *et al.* (1992, 1993); Zhu *et al.* (1992); Wu *et al.* (1992).



Experimental

Crystal data

$[WAg_3IS_4(C_{18}H_{15}P)_3]\cdot 0.45CH_2Cl_2$
M_r = 1587.63
Triclinic, $P\overline{1}$
a = 12.113 (3) Å
b = 13.3231 (14) Å
c = 20.0301 (14) Å
α = 74.671 (8)°
β = 87.659 (11)°
γ = 63.692 (10)°
V = 2783.7 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.97 mm^{-1}
T = 150 (2) K
0.37 × 0.22 × 0.18 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: numerical (*SHELXTL*; Sheldrick, 2005)
T_{min} = 0.321, T_{max} = 0.545
38642 measured reflections
12444 independent reflections
10245 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.068
S = 0.98
12444 reflections
614 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

W—S1	2.2621 (9)	Ag2—S1	2.5631 (10)
W—S2	2.2464 (9)	Ag2—S2	2.5718 (10)
W—S3	2.2423 (10)	Ag2—I	3.0683 (9)
W—S4	2.1440 (11)	Ag2—P2	2.3961 (10)
Ag1—S1	2.5341 (11)	Ag3—S2	2.5892 (11)
Ag1—S3	2.5683 (9)	Ag3—S3	2.6319 (10)
Ag1—I	3.0689 (7)	Ag3—I	3.0231 (5)
Ag1—P1	2.3927 (9)	Ag3—P3	2.4150 (10)
S1—W—S2	111.00 (3)	S2—Ag3—S3	90.19 (3)
S1—W—S3	110.99 (3)	S2—Ag3—I	103.92 (3)
S1—W—S4	107.87 (4)	S2—Ag3—P3	126.86 (3)
S2—W—S3	110.95 (3)	S3—Ag3—I	98.97 (2)
S2—W—S4	107.43 (4)	S3—Ag3—P3	122.69 (3)
S3—W—S4	108.45 (4)	I—Ag3—P3	109.54 (3)
S1—Ag1—S3	93.35 (3)	W—S1—Ag1	76.58 (3)
S1—Ag1—I	99.88 (3)	W—S1—Ag2	75.80 (3)
S1—Ag1—P1	128.00 (3)	Ag1—S1—Ag2	88.04 (3)
S3—Ag1—I	99.25 (2)	W—S2—Ag2	75.89 (3)
S3—Ag1—P1	126.77 (3)	W—S2—Ag3	77.27 (3)
I—Ag1—P1	103.73 (3)	Ag2—S2—Ag3	83.52 (3)
S1—Ag2—S2	92.71 (3)	W—S3—Ag1	76.20 (3)
S1—Ag2—I	99.23 (3)	W—S3—Ag3	76.44 (3)
S1—Ag2—P2	123.93 (3)	Ag1—S3—Ag3	87.30 (3)
S2—Ag2—I	103.11 (3)	Ag1—I—Ag2	70.505 (16)
S2—Ag2—P2	128.24 (3)	Ag1—I—Ag3	72.199 (14)
I—Ag2—P2	104.95 (3)	Ag2—I—Ag3	68.704 (14)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2438).

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supplementary materials

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μ_3-Iodido-tri-μ_3-sulfido-tris[(triphenylphosphine)silver(I)][thioxotungsten(VI)] dichloromethane 0.45-solvate

A. Beheshti, W. Clegg, S. H. Dale and R. Hyvadi

Comment

The title complex was obtained as an unexpected decomposition product in an attempt to prepare a WS_4/Ag/Zn mixed-metal complex containing phosphine and heterocyclic thione ligands. It features a pseudo-cubane WS_3Ag_3I core with a typical geometry involving wide angles at the metal corners and narrow angles at the S and I atoms, giving short W···Ag distances [2.9737 (5)–3.0310 (8) Å] that do not represent formal direct metal-metal bonds.

The W atom has an almost regular tetrahedral coordination geometry, with the terminal W═S bond significantly shorter than the bonds to triply-bridging S atoms. The coordination of the Ag atoms is rather distorted tetrahedral, with the smallest angle in each case between the two Ag—S bonds and the largest angles between Ag—S and Ag—P bonds, as a consequence of the steric demands of the triphenylphosphine ligands.

Very similar structures have been found for related complexes in which one or more of the following substitutions are made: Mo for W, O for the terminal S, Cl or Br for I, pyridyl for one of the phenyl rings on each phosphine ligand (Jin *et al.*, 1999, 2000; Sakane *et al.*, 1996; Wang *et al.*, 2003; Lang *et al.*, 1992, 1993; Zhu *et al.*, 1992; Wu *et al.*, 1992). Some of these are actually isomorphous and probably isostructural with the title complex, although the solvent is water rather than dichloromethane in one case, but coordinates are not available for all of the structures.

Experimental

This compound is an unexpected product in the attempted preparation of $[WS_4Ag(PPh_3)IZn(Diap)_2]$ (Diap = 1,3-diazepane-2-thione). An aqueous solution of $(Diap)_2Zn(OAc)_2{\cdot}H_2O$ (0.05 mmol, 0.023 g) was added to an aqueous solution of $(NH_4)_2[WS_4]$ (0.05 mmol, 0.017 g) in a total volume of 5 ml of water and the mixture was stirred for 2 min. The yellow precipitate was separated by centrifugation and washed with EtOH (2 × 5 ml) and Et_2O (2 × 5 ml). The yellow product, which is soluble in all common organic solvents, was dissolved in CH_2Cl_2 (10 ml) and solid AgI (0.05 mmol, 0.011 g) and PPh_3 (0.05 mmol, 0.013 g) were added. The mixture was stirred for 30 min and then filtered. The filtrate was evaporated under vacuum. The residue was washed with diethyl ether (2 × 5 ml) and dried *in vacuo* to give a yellow powder. Single crystals were obtained by slow diffusion of diethyl ether into an acetone solution of the complex. On leaving the solution to stand in a refrigerator overnight, air-stable yellow crystals were deposited.

The FT—IR spectrum in the range 4000–400 cm^{-1} shows all the expected strong phosphine bands, which remain practically unshifted from those of the uncomplexed ligand. The spectrum also displays a doublet at 419.4 and 438.8 cm^{-1}, which is attributed to ν(W—μ_3-S) vibrations. A strong band at 510 cm^{-1} is due to the δ(C—H) vibrations of the PPh_3 ligands It is difficult to identify features due to the W—S(terminal) and Ag—P absorptions, because the PPh_3 ligands give rise to a strong band in the same positions as expected for these features. The electronic absorption spectrum of the complex in

DMF solution appears to be mainly of intraligand character, presenting two broad bands with maxima at 291 and 401.5 nm. These absorptions can be assigned as charge-transfer bands of the type (π)S→ (*d*)W arising from the WS_4 group; these are red-shifted compared to the free $[WS_4]^{2-}$ anion.

Refinement

Hydrogen atoms were positioned geometrically and refined with a riding model, with C—H = 0.95 or 0.99 Å and with $U_{iso} = 1.2U_{eq}$(C). The dichloromethane solvent molecule is disordered equally over two positions close to an inversion centre, sharing the Cl atom sites; no restraints were used, and the anisotropic displacement parameters indicate that the disorder is actually more complicated. The largest residual electron density peaks are close to W and Cl atoms.

Figures

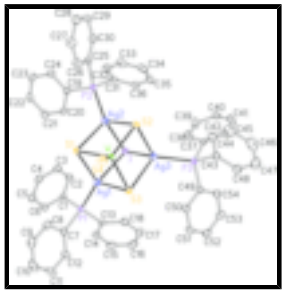


Fig. 1. The molecular structure with atom labels and 40% probability ellipsoids for non-H atoms. H atoms and the solvent molecule have been omitted.

μ_3-Iodido-tri-μ_3-sulfido- tris[(triphenylphosphine)silver(I)][thioxotungsten(VI)] dichloromethane 0.45-solvate

Crystal data

$[WAg_3IS_4(C_{18}H_{15}P)_3]\cdot 0.45CH_2Cl_2$	$Z = 2$
$M_r = 1587.63$	$F_{000} = 1530$
Triclinic, $P\overline{1}$	$D_x = 1.894$ Mg m^{-3}
$a = 12.113$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 13.3231$ (14) Å	Cell parameters from 643 reflections
$c = 20.0301$ (14) Å	$\theta = 2.5$–27.5°
$\alpha = 74.671$ (8)°	$\mu = 3.97$ mm^{-1}
$\beta = 87.659$ (11)°	$T = 150$ (2) K
$\gamma = 63.692$ (10)°	Block, yellow
$V = 2783.7$ (8) Å^3	0.37 × 0.22 × 0.18 mm

Data collection

Nonius KappaCCD diffractometer	12444 independent reflections
Radiation source: fine-focus sealed tube	10245 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.049$
$T = 150(2)$ K	$\theta_{max} = 27.5^\circ$

φ and ω scans

Absorption correction: numerical (SHELXTL; Sheldrick, 2005)

T_{min} = 0.321, T_{max} = 0.545

38642 measured reflections

θ_{min} = 4.4°

h = −15→15

k = −16→17

l = −25→26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.028

$wR(F^2)$ = 0.068

S = 0.98

12444 reflections

614 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 1.8123P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 1.21 e Å^{-3}

$\Delta\rho_{min}$ = −0.98 e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
W	0.105460 (12)	0.535347 (11)	0.148656 (7)	0.01491 (4)	
Ag1	0.25207 (3)	0.58341 (3)	0.240876 (15)	0.02614 (7)	
Ag2	0.17124 (3)	0.35043 (2)	0.282604 (15)	0.03036 (8)	
Ag3	0.37164 (3)	0.35425 (2)	0.156496 (17)	0.02844 (7)	
S1	0.04814 (8)	0.57272 (8)	0.25178 (5)	0.01983 (18)	
S2	0.16114 (9)	0.34801 (8)	0.15507 (5)	0.02232 (19)	
S3	0.25794 (8)	0.58312 (7)	0.11261 (5)	0.01902 (18)	
S4	−0.05180 (9)	0.63984 (9)	0.07374 (5)	0.0313 (2)	
I	0.43103 (2)	0.326826 (19)	0.307325 (12)	0.02289 (6)	
P1	0.32368 (8)	0.68707 (8)	0.29432 (5)	0.01763 (19)	
C1	0.3168 (3)	0.6609 (3)	0.38846 (19)	0.0203 (7)	
C2	0.3521 (3)	0.5466 (3)	0.42839 (19)	0.0242 (8)	
H2	0.3747	0.4864	0.4061	0.029*	
C3	0.3546 (4)	0.5203 (3)	0.5001 (2)	0.0300 (9)	
H3	0.3802	0.4419	0.5266	0.036*	
C4	0.3204 (4)	0.6067 (4)	0.5335 (2)	0.0315 (9)	
H4	0.3211	0.5884	0.5827	0.038*	
C5	0.2849 (4)	0.7202 (4)	0.4944 (2)	0.0335 (10)	
H5	0.2612	0.7803	0.5169	0.040*	
C6	0.2836 (4)	0.7473 (3)	0.4220 (2)	0.0268 (8)	
H6	0.2599	0.8255	0.3957	0.032*	
C7	0.2375 (3)	0.8447 (3)	0.26030 (19)	0.0227 (8)	
C8	0.1089 (4)	0.8910 (4)	0.2542 (2)	0.0358 (10)	
H8	0.0708	0.8406	0.2657	0.043*	
C9	0.0363 (4)	1.0109 (4)	0.2313 (2)	0.0454 (12)	

H9	−0.0513	1.0423	0.2284	0.054*
C10	0.0915 (5)	1.0837 (4)	0.2129 (2)	0.0433 (12)
H10	0.0419	1.1657	0.1978	0.052*
C11	0.2174 (5)	1.0387 (3)	0.2161 (2)	0.0400 (11)
H11	0.2547	1.0895	0.2018	0.048*
C12	0.2914 (4)	0.9193 (3)	0.2400 (2)	0.0299 (9)
H12	0.3789	0.8889	0.2424	0.036*
C13	0.4860 (3)	0.6514 (3)	0.28289 (18)	0.0183 (7)
C14	0.5505 (4)	0.6868 (3)	0.32088 (19)	0.0252 (8)
H14	0.5108	0.7261	0.3547	0.030*
C15	0.6706 (4)	0.6648 (4)	0.3094 (2)	0.0336 (10)
H15	0.7132	0.6908	0.3341	0.040*
C16	0.7295 (4)	0.6042 (4)	0.2612 (2)	0.0398 (11)
H16	0.8124	0.5893	0.2530	0.048*
C17	0.6687 (4)	0.5656 (4)	0.2255 (2)	0.0361 (10)
H17	0.7103	0.5227	0.1935	0.043*
C18	0.5467 (3)	0.5893 (3)	0.2362 (2)	0.0270 (8)
H18	0.5047	0.5628	0.2114	0.032*
P2	0.14681 (9)	0.22050 (8)	0.38378 (5)	0.02021 (19)
C19	0.1090 (3)	0.2784 (3)	0.45942 (18)	0.0209 (8)
C20	0.1687 (3)	0.3413 (3)	0.47205 (19)	0.0242 (8)
H20	0.2253	0.3547	0.4410	0.029*
C21	0.1456 (4)	0.3843 (3)	0.5299 (2)	0.0290 (9)
H21	0.1859	0.4275	0.5381	0.035*
C22	0.0646 (4)	0.3645 (3)	0.5754 (2)	0.0294 (9)
H22	0.0499	0.3934	0.6151	0.035*
C23	0.0042 (4)	0.3028 (3)	0.5636 (2)	0.0306 (9)
H23	−0.0519	0.2896	0.5950	0.037*
C24	0.0260 (4)	0.2599 (3)	0.5053 (2)	0.0272 (8)
H24	−0.0159	0.2180	0.4970	0.033*
C25	0.0217 (3)	0.1831 (3)	0.37216 (18)	0.0208 (8)
C26	−0.0861 (4)	0.2707 (3)	0.3318 (2)	0.0302 (9)
H26	−0.0904	0.3449	0.3095	0.036*
C27	−0.1862 (4)	0.2500 (4)	0.3242 (2)	0.0349 (10)
H27	−0.2592	0.3101	0.2969	0.042*
C28	−0.1806 (4)	0.1417 (4)	0.3563 (2)	0.0331 (10)
H28	−0.2500	0.1278	0.3515	0.040*
C29	−0.0741 (4)	0.0546 (4)	0.3949 (2)	0.0336 (10)
H29	−0.0697	−0.0200	0.4160	0.040*
C30	0.0277 (4)	0.0744 (3)	0.4037 (2)	0.0263 (8)
H30	0.1004	0.0139	0.4310	0.032*
C31	0.2853 (3)	0.0832 (3)	0.4146 (2)	0.0222 (8)
C32	0.3116 (4)	0.0162 (3)	0.4846 (2)	0.0302 (9)
H32	0.2557	0.0424	0.5179	0.036*
C33	0.4182 (4)	−0.0872 (4)	0.5048 (2)	0.0388 (11)
H33	0.4352	−0.1327	0.5519	0.047*
C34	0.4995 (4)	−0.1242 (4)	0.4570 (3)	0.0440 (12)
H34	0.5724	−0.1959	0.4713	0.053*
C35	0.4775 (4)	−0.0600 (4)	0.3889 (3)	0.0406 (11)

H35	0.5354	−0.0868	0.3565	0.049*	
C36	0.3702 (4)	0.0449 (3)	0.3669 (2)	0.0289 (9)	
H36	0.3551	0.0899	0.3198	0.035*	
P3	0.55628 (8)	0.23800 (8)	0.10917 (5)	0.02003 (19)	
C37	0.6526 (3)	0.0897 (3)	0.16250 (19)	0.0194 (7)	
C38	0.6651 (4)	0.0684 (3)	0.2341 (2)	0.0330 (10)	
H38	0.6211	0.1305	0.2544	0.040*	
C39	0.7405 (4)	−0.0420 (3)	0.2768 (2)	0.0363 (10)	
H39	0.7479	−0.0551	0.3258	0.044*	
C40	0.8041 (4)	−0.1317 (3)	0.2475 (2)	0.0289 (9)	
H40	0.8568	−0.2070	0.2763	0.035*	
C41	0.7920 (4)	−0.1133 (3)	0.1771 (2)	0.0432 (12)	
H41	0.8357	−0.1761	0.1573	0.052*	
C42	0.7158 (4)	−0.0028 (3)	0.1343 (2)	0.0387 (11)	
H42	0.7072	0.0091	0.0855	0.046*	
C43	0.5242 (3)	0.2135 (3)	0.02780 (19)	0.0227 (8)	
C44	0.4232 (4)	0.1924 (3)	0.0225 (2)	0.0329 (9)	
H44	0.3703	0.1959	0.0591	0.039*	
C45	0.3990 (4)	0.1662 (4)	−0.0364 (3)	0.0433 (11)	
H45	0.3303	0.1508	−0.0398	0.052*	
C46	0.4756 (5)	0.1626 (4)	−0.0901 (3)	0.0478 (12)	
H46	0.4595	0.1440	−0.1301	0.057*	
C47	0.5745 (5)	0.1857 (4)	−0.0858 (2)	0.0435 (11)	
H47	0.6257	0.1843	−0.1231	0.052*	
C48	0.5998 (4)	0.2113 (3)	−0.0268 (2)	0.0307 (9)	
H48	0.6683	0.2271	−0.0237	0.037*	
C49	0.6616 (3)	0.3046 (3)	0.09070 (18)	0.0217 (8)	
C50	0.6130 (4)	0.4248 (3)	0.0786 (2)	0.0274 (8)	
H50	0.5268	0.4701	0.0800	0.033*	
C51	0.6905 (4)	0.4789 (3)	0.0644 (2)	0.0331 (9)	
H51	0.6564	0.5610	0.0559	0.040*	
C52	0.8155 (4)	0.4147 (4)	0.0625 (2)	0.0326 (9)	
H52	0.8677	0.4521	0.0535	0.039*	
C53	0.8652 (4)	0.2947 (4)	0.0739 (2)	0.0312 (9)	
H53	0.9513	0.2500	0.0718	0.037*	
C54	0.7887 (3)	0.2403 (3)	0.0882 (2)	0.0280 (9)	
H54	0.8232	0.1582	0.0965	0.034*	
Cl	1.0901 (3)	0.0109 (3)	0.0356 (2)	0.182 (3)	0.898 (9)
C55	0.9850 (12)	0.0868 (12)	−0.0452 (9)	0.092 (6)	0.449 (4)
H55A	0.9249	0.1672	−0.0459	0.111*	0.449 (4)
H55B	1.0308	0.0882	−0.0873	0.111*	0.449 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W	0.01416 (8)	0.01395 (7)	0.01676 (7)	−0.00668 (6)	0.00146 (5)	−0.00376 (5)
Ag1	0.02735 (16)	0.03518 (17)	0.02890 (16)	−0.02200 (14)	0.00552 (12)	−0.01526 (13)
Ag2	0.04511 (19)	0.02228 (15)	0.02184 (15)	−0.01689 (14)	0.00866 (13)	−0.00086 (12)

Ag3	0.02171 (16)	0.02078 (15)	0.03969 (18)	−0.00569 (12)	0.01081 (13)	−0.01155 (13)
S1	0.0169 (4)	0.0212 (4)	0.0242 (5)	−0.0092 (4)	0.0078 (3)	−0.0104 (4)
S2	0.0280 (5)	0.0185 (4)	0.0258 (5)	−0.0137 (4)	0.0043 (4)	−0.0089 (4)
S3	0.0196 (5)	0.0173 (4)	0.0197 (4)	−0.0094 (4)	0.0049 (3)	−0.0029 (3)
S4	0.0236 (5)	0.0308 (5)	0.0320 (6)	−0.0084 (4)	−0.0086 (4)	−0.0021 (4)
I	0.02200 (13)	0.01956 (12)	0.02312 (13)	−0.00603 (10)	0.00018 (9)	−0.00527 (9)
P1	0.0166 (5)	0.0186 (5)	0.0205 (5)	−0.0101 (4)	0.0028 (3)	−0.0061 (4)
C1	0.0201 (19)	0.0212 (18)	0.0222 (19)	−0.0111 (15)	0.0039 (14)	−0.0070 (15)
C2	0.026 (2)	0.0240 (19)	0.024 (2)	−0.0136 (16)	0.0041 (15)	−0.0056 (16)
C3	0.028 (2)	0.030 (2)	0.027 (2)	−0.0133 (18)	0.0026 (16)	0.0009 (17)
C4	0.030 (2)	0.045 (3)	0.021 (2)	−0.018 (2)	0.0048 (16)	−0.0080 (18)
C5	0.039 (2)	0.041 (2)	0.028 (2)	−0.020 (2)	0.0113 (18)	−0.0184 (19)
C6	0.031 (2)	0.025 (2)	0.027 (2)	−0.0135 (17)	0.0047 (16)	−0.0111 (16)
C7	0.026 (2)	0.0211 (19)	0.0200 (19)	−0.0088 (16)	0.0016 (15)	−0.0069 (15)
C8	0.024 (2)	0.037 (2)	0.034 (2)	−0.0096 (19)	0.0050 (17)	0.0030 (19)
C9	0.029 (2)	0.041 (3)	0.037 (3)	0.005 (2)	0.0020 (19)	−0.002 (2)
C10	0.052 (3)	0.021 (2)	0.036 (3)	0.002 (2)	−0.008 (2)	−0.0063 (19)
C11	0.059 (3)	0.021 (2)	0.038 (3)	−0.018 (2)	−0.010 (2)	−0.0034 (18)
C12	0.034 (2)	0.023 (2)	0.034 (2)	−0.0143 (18)	−0.0036 (18)	−0.0066 (17)
C13	0.0166 (18)	0.0184 (17)	0.0188 (18)	−0.0097 (15)	0.0005 (13)	0.0001 (14)
C14	0.028 (2)	0.028 (2)	0.0212 (19)	−0.0157 (17)	−0.0014 (15)	−0.0048 (16)
C15	0.028 (2)	0.039 (2)	0.036 (2)	−0.022 (2)	−0.0080 (18)	−0.0006 (19)
C16	0.018 (2)	0.044 (3)	0.050 (3)	−0.014 (2)	0.0038 (19)	−0.001 (2)
C17	0.027 (2)	0.039 (2)	0.042 (3)	−0.014 (2)	0.0114 (19)	−0.014 (2)
C18	0.025 (2)	0.031 (2)	0.027 (2)	−0.0131 (18)	0.0035 (16)	−0.0107 (17)
P2	0.0224 (5)	0.0175 (5)	0.0189 (5)	−0.0093 (4)	0.0024 (4)	−0.0016 (4)
C19	0.0211 (19)	0.0179 (18)	0.0204 (19)	−0.0075 (15)	0.0013 (14)	−0.0025 (14)
C20	0.023 (2)	0.026 (2)	0.023 (2)	−0.0125 (17)	0.0043 (15)	−0.0042 (16)
C21	0.028 (2)	0.027 (2)	0.031 (2)	−0.0122 (18)	−0.0014 (17)	−0.0075 (17)
C22	0.028 (2)	0.028 (2)	0.022 (2)	−0.0044 (17)	0.0003 (16)	−0.0069 (16)
C23	0.026 (2)	0.036 (2)	0.027 (2)	−0.0132 (18)	0.0099 (16)	−0.0074 (18)
C24	0.026 (2)	0.029 (2)	0.030 (2)	−0.0164 (18)	0.0043 (16)	−0.0064 (17)
C25	0.025 (2)	0.0205 (18)	0.0159 (18)	−0.0101 (16)	−0.0001 (14)	−0.0042 (14)
C26	0.030 (2)	0.023 (2)	0.031 (2)	−0.0094 (17)	−0.0072 (17)	0.0006 (17)
C27	0.029 (2)	0.033 (2)	0.037 (3)	−0.0099 (19)	−0.0058 (18)	−0.0071 (19)
C28	0.029 (2)	0.043 (3)	0.037 (2)	−0.021 (2)	0.0017 (18)	−0.017 (2)
C29	0.041 (3)	0.032 (2)	0.037 (2)	−0.026 (2)	0.0030 (19)	−0.0072 (19)
C30	0.026 (2)	0.022 (2)	0.027 (2)	−0.0113 (17)	−0.0017 (16)	−0.0003 (16)
C31	0.0197 (19)	0.0176 (18)	0.028 (2)	−0.0093 (15)	−0.0018 (15)	−0.0025 (15)
C32	0.030 (2)	0.027 (2)	0.030 (2)	−0.0143 (18)	−0.0019 (17)	0.0007 (17)
C33	0.037 (3)	0.026 (2)	0.045 (3)	−0.012 (2)	−0.019 (2)	0.0029 (19)
C34	0.027 (2)	0.021 (2)	0.078 (4)	−0.0050 (19)	−0.012 (2)	−0.012 (2)
C35	0.031 (2)	0.036 (2)	0.067 (3)	−0.017 (2)	0.012 (2)	−0.030 (2)
C36	0.027 (2)	0.024 (2)	0.037 (2)	−0.0119 (17)	0.0080 (17)	−0.0120 (17)
P3	0.0187 (5)	0.0153 (4)	0.0220 (5)	−0.0040 (4)	0.0030 (4)	−0.0053 (4)
C37	0.0191 (18)	0.0171 (17)	0.0217 (19)	−0.0083 (15)	0.0048 (14)	−0.0052 (14)
C38	0.038 (2)	0.0189 (19)	0.028 (2)	0.0028 (17)	−0.0044 (18)	−0.0102 (17)
C39	0.042 (3)	0.030 (2)	0.021 (2)	−0.0032 (19)	−0.0021 (18)	−0.0040 (17)
C40	0.029 (2)	0.0180 (19)	0.034 (2)	−0.0092 (17)	−0.0018 (17)	−0.0004 (16)

C41	0.056 (3)	0.018 (2)	0.040 (3)	0.001 (2)	−0.002 (2)	−0.0139 (19)
C42	0.056 (3)	0.021 (2)	0.027 (2)	−0.004 (2)	0.003 (2)	−0.0098 (17)
C43	0.0198 (19)	0.0166 (18)	0.023 (2)	−0.0013 (15)	−0.0009 (15)	−0.0047 (15)
C44	0.031 (2)	0.027 (2)	0.038 (2)	−0.0101 (18)	0.0007 (18)	−0.0077 (18)
C45	0.039 (3)	0.045 (3)	0.049 (3)	−0.018 (2)	−0.006 (2)	−0.018 (2)
C46	0.059 (3)	0.048 (3)	0.031 (3)	−0.017 (3)	−0.010 (2)	−0.013 (2)
C47	0.053 (3)	0.052 (3)	0.023 (2)	−0.021 (2)	0.005 (2)	−0.011 (2)
C48	0.034 (2)	0.034 (2)	0.023 (2)	−0.0154 (19)	0.0020 (17)	−0.0057 (17)
C49	0.0218 (19)	0.0220 (19)	0.0184 (18)	−0.0079 (16)	0.0012 (14)	−0.0043 (15)
C50	0.027 (2)	0.0207 (19)	0.031 (2)	−0.0076 (17)	0.0029 (16)	−0.0066 (16)
C51	0.042 (3)	0.023 (2)	0.035 (2)	−0.0167 (19)	0.0056 (19)	−0.0067 (17)
C52	0.045 (3)	0.042 (2)	0.022 (2)	−0.030 (2)	0.0044 (18)	−0.0062 (18)
C53	0.023 (2)	0.037 (2)	0.030 (2)	−0.0130 (18)	−0.0003 (16)	−0.0020 (18)
C54	0.024 (2)	0.025 (2)	0.033 (2)	−0.0100 (17)	0.0039 (16)	−0.0072 (17)
Cl	0.096 (2)	0.203 (4)	0.203 (4)	0.028 (2)	−0.019 (2)	−0.152 (3)
C55	0.042 (8)	0.072 (10)	0.119 (14)	−0.006 (7)	0.044 (9)	0.001 (9)

Geometric parameters (Å, °)

W—S1	2.2621 (9)	C24—H24	0.950
W—S2	2.2464 (9)	C25—C26	1.399 (5)
W—S3	2.2423 (10)	C25—C30	1.389 (5)
W—S4	2.1440 (11)	C26—H26	0.950
Ag1—S1	2.5341 (11)	C26—C27	1.380 (6)
Ag1—S3	2.5683 (9)	C27—H27	0.950
Ag1—I	3.0689 (7)	C27—C28	1.388 (6)
Ag1—P1	2.3927 (9)	C28—H28	0.950
Ag2—S1	2.5631 (10)	C28—C29	1.375 (6)
Ag2—S2	2.5718 (10)	C29—H29	0.950
Ag2—I	3.0683 (9)	C29—C30	1.396 (5)
Ag2—P2	2.3961 (10)	C30—H30	0.950
Ag3—S2	2.5892 (11)	C31—C32	1.410 (5)
Ag3—S3	2.6319 (10)	C31—C36	1.394 (5)
Ag3—I	3.0231 (5)	C32—H32	0.950
Ag3—P3	2.4150 (10)	C32—C33	1.378 (6)
P1—C1	1.830 (4)	C33—H33	0.950
P1—C7	1.823 (4)	C33—C34	1.368 (7)
P1—C13	1.827 (4)	C34—H34	0.950
C1—C2	1.396 (5)	C34—C35	1.370 (7)
C1—C6	1.385 (5)	C35—H35	0.950
C2—H2	0.950	C35—C36	1.395 (6)
C2—C3	1.383 (5)	C36—H36	0.950
C3—H3	0.950	P3—C37	1.830 (4)
C3—C4	1.381 (5)	P3—C43	1.833 (4)
C4—H4	0.950	P3—C49	1.829 (4)
C4—C5	1.382 (6)	C37—C38	1.387 (5)
C5—H5	0.950	C37—C42	1.386 (5)
C5—C6	1.396 (5)	C38—H38	0.950
C6—H6	0.950	C38—C39	1.392 (5)

C7—C8	1.395 (5)	C39—H39	0.950
C7—C12	1.386 (5)	C39—C40	1.373 (5)
C8—H8	0.950	C40—H40	0.950
C8—C9	1.390 (6)	C40—C41	1.368 (6)
C9—H9	0.950	C41—H41	0.950
C9—C10	1.375 (7)	C41—C42	1.397 (6)
C10—H10	0.950	C42—H42	0.950
C10—C11	1.366 (7)	C43—C44	1.385 (5)
C11—H11	0.950	C43—C48	1.395 (5)
C11—C12	1.389 (5)	C44—H44	0.950
C12—H12	0.950	C44—C45	1.391 (6)
C13—C14	1.405 (5)	C45—H45	0.950
C13—C18	1.384 (5)	C45—C46	1.387 (7)
C14—H14	0.950	C46—H46	0.950
C14—C15	1.373 (5)	C46—C47	1.374 (7)
C15—H15	0.950	C47—H47	0.950
C15—C16	1.392 (6)	C47—C48	1.394 (6)
C16—H16	0.950	C48—H48	0.950
C16—C17	1.376 (6)	C49—C50	1.393 (5)
C17—H17	0.950	C49—C54	1.397 (5)
C17—C18	1.389 (5)	C50—H50	0.950
C18—H18	0.950	C50—C51	1.397 (5)
P2—C19	1.830 (4)	C51—H51	0.950
P2—C25	1.833 (4)	C51—C52	1.375 (6)
P2—C31	1.819 (4)	C52—H52	0.950
C19—C20	1.397 (5)	C52—C53	1.392 (6)
C19—C24	1.393 (5)	C53—H53	0.950
C20—H20	0.950	C53—C54	1.390 (5)
C20—C21	1.390 (5)	C54—H54	0.950
C21—H21	0.950	Cl—C55	1.851 (17)
C21—C22	1.375 (5)	Cl—C55^{i}	1.862 (16)
C22—H22	0.950	C55—Cl^{i}	1.862 (16)
C22—C23	1.384 (6)	C55—H55A	0.990
C23—H23	0.950	C55—H55B	0.990
C23—C24	1.397 (5)		
S1—W—S2	111.00 (3)	C21—C22—C23	120.4 (4)
S1—W—S3	110.99 (3)	H22—C22—C23	119.8
S1—W—S4	107.87 (4)	C22—C23—H23	120.0
S2—W—S3	110.95 (3)	C22—C23—C24	119.9 (4)
S2—W—S4	107.43 (4)	H23—C23—C24	120.0
S3—W—S4	108.45 (4)	C19—C24—C23	120.1 (3)
S1—Ag1—S3	93.35 (3)	C19—C24—H24	120.0
S1—Ag1—I	99.88 (3)	C23—C24—H24	120.0
S1—Ag1—P1	128.00 (3)	P2—C25—C26	117.6 (3)
S3—Ag1—I	99.25 (2)	P2—C25—C30	123.1 (3)
S3—Ag1—P1	126.77 (3)	C26—C25—C30	119.3 (3)
I—Ag1—P1	103.73 (3)	C25—C26—H26	119.8
S1—Ag2—S2	92.71 (3)	C25—C26—C27	120.4 (4)

S1—Ag2—I	99.23 (3)	H26—C26—C27	119.8
S1—Ag2—P2	123.93 (3)	C26—C27—H27	119.9
S2—Ag2—I	103.11 (3)	C26—C27—C28	120.2 (4)
S2—Ag2—P2	128.24 (3)	H27—C27—C28	119.9
I—Ag2—P2	104.95 (3)	C27—C28—H28	120.2
S2—Ag3—S3	90.19 (3)	C27—C28—C29	119.6 (4)
S2—Ag3—I	103.92 (3)	H28—C28—C29	120.2
S2—Ag3—P3	126.86 (3)	C28—C29—H29	119.6
S3—Ag3—I	98.97 (2)	C28—C29—C30	120.9 (4)
S3—Ag3—P3	122.69 (3)	H29—C29—C30	119.6
I—Ag3—P3	109.54 (3)	C25—C30—C29	119.5 (4)
W—S1—Ag1	76.58 (3)	C25—C30—H30	120.2
W—S1—Ag2	75.80 (3)	C29—C30—H30	120.2
Ag1—S1—Ag2	88.04 (3)	P2—C31—C32	122.9 (3)
W—S2—Ag2	75.89 (3)	P2—C31—C36	118.2 (3)
W—S2—Ag3	77.27 (3)	C32—C31—C36	119.0 (3)
Ag2—S2—Ag3	83.52 (3)	C31—C32—H32	119.9
W—S3—Ag1	76.20 (3)	C31—C32—C33	120.1 (4)
W—S3—Ag3	76.44 (3)	H32—C32—C33	119.9
Ag1—S3—Ag3	87.30 (3)	C32—C33—H33	120.0
Ag1—I—Ag2	70.505 (16)	C32—C33—C34	120.0 (4)
Ag1—I—Ag3	72.199 (14)	H33—C33—C34	120.0
Ag2—I—Ag3	68.704 (14)	C33—C34—H34	119.4
Ag1—P1—C1	116.19 (11)	C33—C34—C35	121.2 (4)
Ag1—P1—C7	113.08 (12)	H34—C34—C35	119.4
Ag1—P1—C13	112.69 (12)	C34—C35—H35	120.0
C1—P1—C7	104.13 (16)	C34—C35—C36	120.1 (4)
C1—P1—C13	103.49 (16)	H35—C35—C36	120.0
C7—P1—C13	106.22 (16)	C31—C36—C35	119.6 (4)
P1—C1—C2	117.8 (3)	C31—C36—H36	120.2
P1—C1—C6	123.5 (3)	C35—C36—H36	120.2
C2—C1—C6	118.6 (3)	Ag3—P3—C37	117.03 (12)
C1—C2—H2	119.7	Ag3—P3—C43	113.15 (12)
C1—C2—C3	120.6 (4)	Ag3—P3—C49	112.36 (12)
H2—C2—C3	119.7	C37—P3—C43	102.27 (16)
C2—C3—H3	119.6	C37—P3—C49	104.46 (16)
C2—C3—C4	120.7 (4)	C43—P3—C49	106.46 (17)
H3—C3—C4	119.6	P3—C37—C38	119.1 (3)
C3—C4—H4	120.4	P3—C37—C42	122.7 (3)
C3—C4—C5	119.2 (4)	C38—C37—C42	118.2 (3)
H4—C4—C5	120.4	C37—C38—H38	119.3
C4—C5—H5	119.7	C37—C38—C39	121.4 (4)
C4—C5—C6	120.5 (4)	H38—C38—C39	119.3
H5—C5—C6	119.7	C38—C39—H39	120.4
C1—C6—C5	120.4 (4)	C38—C39—C40	119.3 (4)
C1—C6—H6	119.8	H39—C39—C40	120.4
C5—C6—H6	119.8	C39—C40—H40	119.8
P1—C7—C8	116.6 (3)	C39—C40—C41	120.4 (4)
P1—C7—C12	124.4 (3)	H40—C40—C41	119.8

C8—C7—C12	119.0 (4)	C40—C41—H41	119.9
C7—C8—H8	119.9	C40—C41—C42	120.3 (4)
C7—C8—C9	120.2 (4)	H41—C41—C42	119.9
H8—C8—C9	119.9	C37—C42—C41	120.3 (4)
C8—C9—H9	120.0	C37—C42—H42	119.8
C8—C9—C10	119.9 (4)	C41—C42—H42	119.8
H9—C9—C10	120.0	P3—C43—C44	117.7 (3)
C9—C10—H10	119.9	P3—C43—C48	122.4 (3)
C9—C10—C11	120.2 (4)	C44—C43—C48	119.8 (4)
H10—C10—C11	119.9	C43—C44—H44	120.0
C10—C11—H11	119.6	C43—C44—C45	120.1 (4)
C10—C11—C12	120.7 (4)	H44—C44—C45	120.0
H11—C11—C12	119.6	C44—C45—H45	120.1
C7—C12—C11	119.9 (4)	C44—C45—C46	119.7 (4)
C7—C12—H12	120.0	H45—C45—C46	120.1
C11—C12—H12	120.0	C45—C46—H46	119.7
P1—C13—C14	120.8 (3)	C45—C46—C47	120.5 (4)
P1—C13—C18	119.9 (3)	H46—C46—C47	119.7
C14—C13—C18	119.3 (3)	C46—C47—H47	120.0
C13—C14—H14	119.8	C46—C47—C48	120.0 (4)
C13—C14—C15	120.3 (4)	H47—C47—C48	120.0
H14—C14—C15	119.8	C43—C48—C47	119.8 (4)
C14—C15—H15	120.2	C43—C48—H48	120.1
C14—C15—C16	119.6 (4)	C47—C48—H48	120.1
H15—C15—C16	120.2	P3—C49—C50	118.5 (3)
C15—C16—H16	119.7	P3—C49—C54	122.9 (3)
C15—C16—C17	120.6 (4)	C50—C49—C54	118.6 (3)
H16—C16—C17	119.7	C49—C50—H50	119.9
C16—C17—H17	120.0	C49—C50—C51	120.2 (4)
C16—C17—C18	120.0 (4)	H50—C50—C51	119.9
H17—C17—C18	120.0	C50—C51—H51	119.6
C13—C18—C17	120.2 (4)	C50—C51—C52	120.8 (4)
C13—C18—H18	119.9	H51—C51—C52	119.6
C17—C18—H18	119.9	C51—C52—H52	120.2
Ag2—P2—C19	114.01 (12)	C51—C52—C53	119.7 (4)
Ag2—P2—C25	113.98 (12)	H52—C52—C53	120.2
Ag2—P2—C31	113.57 (12)	C52—C53—H53	120.1
C19—P2—C25	103.73 (16)	C52—C53—C54	119.9 (4)
C19—P2—C31	104.17 (17)	H53—C53—C54	120.1
C25—P2—C31	106.36 (16)	C49—C54—C53	120.9 (4)
P2—C19—C20	118.0 (3)	C49—C54—H54	119.6
P2—C19—C24	122.7 (3)	C53—C54—H54	119.6
C20—C19—C24	119.2 (3)	C55—Cl—C55^{i}	81.4 (7)
C19—C20—H20	119.9	Cl—C55—Cl^{i}	98.6 (7)
C19—C20—C21	120.2 (3)	Cl—C55—H55A	112.1
H20—C20—C21	119.9	Cl^{i}—C55—H55A	112.1
C20—C21—H21	119.9	Cl—C55—H55B	112.1
C20—C21—C22	120.3 (4)	Cl^{i}—C55—H55B	112.1

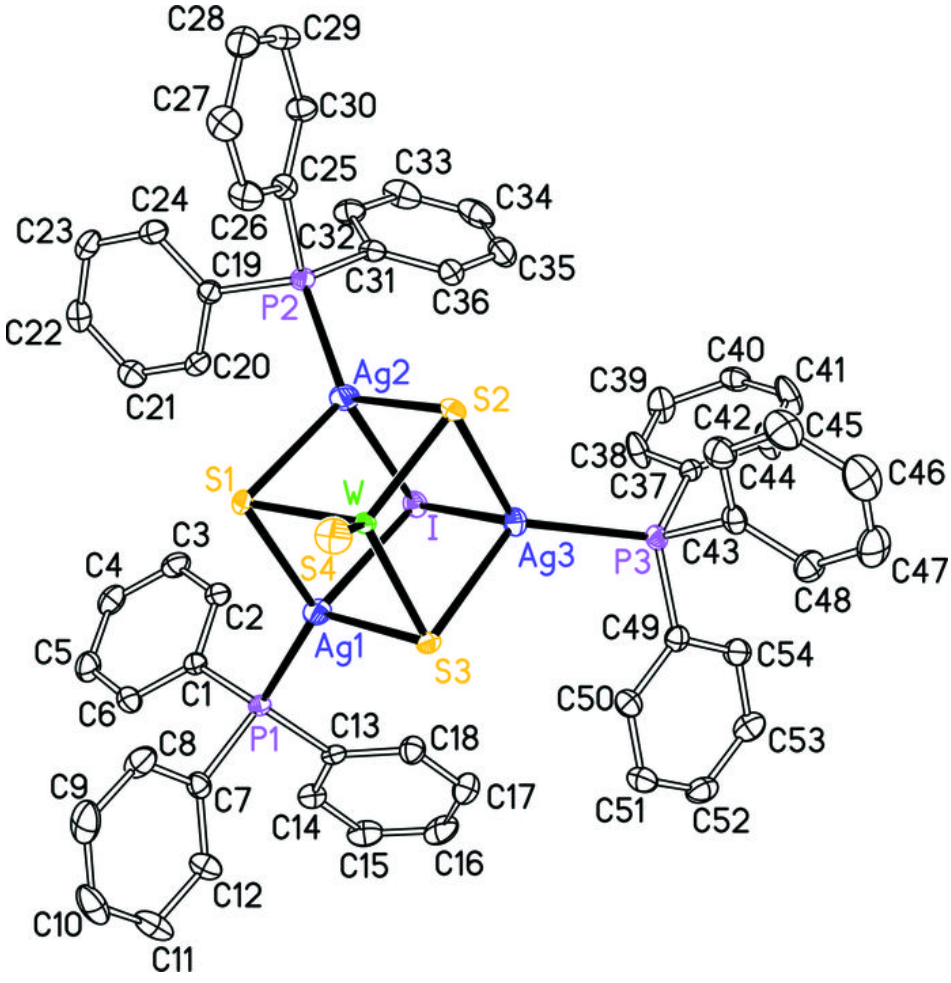
H21—C21—C22	119.9	H55A—C55—H55B	109.7
C21—C22—H22	119.8		
S2—W—S1—Ag1	109.50 (3)	C7—P1—C13—C14	67.3 (3)
S2—W—S1—Ag2	18.11 (4)	C7—P1—C13—C18	−112.4 (3)
S3—W—S1—Ag1	−14.38 (3)	P1—C13—C14—C15	−176.7 (3)
S3—W—S1—Ag2	−105.76 (3)	C18—C13—C14—C15	3.1 (5)
S4—W—S1—Ag1	−133.06 (3)	C13—C14—C15—C16	−1.8 (6)
S4—W—S1—Ag2	135.56 (3)	C14—C15—C16—C17	−0.4 (6)
S3—Ag1—S1—W	11.70 (3)	C15—C16—C17—C18	1.5 (7)
S3—Ag1—S1—Ag2	87.57 (3)	P1—C13—C18—C17	177.7 (3)
I—Ag1—S1—W	−88.30 (2)	C14—C13—C18—C17	−2.1 (6)
I—Ag1—S1—Ag2	−12.43 (2)	C16—C17—C18—C13	−0.2 (6)
P1—Ag1—S1—W	155.48 (3)	S1—Ag2—P2—C19	−33.44 (14)
P1—Ag1—S1—Ag2	−128.65 (4)	S1—Ag2—P2—C25	85.41 (13)
S2—Ag2—S1—W	−14.70 (3)	S1—Ag2—P2—C31	−152.55 (13)
S2—Ag2—S1—Ag1	−91.35 (3)	S2—Ag2—P2—C19	−160.48 (13)
I—Ag2—S1—W	89.05 (2)	S2—Ag2—P2—C25	−41.64 (14)
I—Ag2—S1—Ag1	12.41 (3)	S2—Ag2—P2—C31	80.40 (14)
P2—Ag2—S1—W	−155.83 (3)	I—Ag2—P2—C19	78.89 (13)
P2—Ag2—S1—Ag1	127.52 (4)	I—Ag2—P2—C25	−162.27 (13)
S1—W—S2—Ag2	−18.04 (4)	I—Ag2—P2—C31	−40.23 (13)
S1—W—S2—Ag3	−104.46 (3)	Ag2—P2—C19—C20	−40.0 (3)
S3—W—S2—Ag2	105.85 (3)	Ag2—P2—C19—C24	141.6 (3)
S3—W—S2—Ag3	19.43 (4)	C25—P2—C19—C20	−164.6 (3)
S4—W—S2—Ag2	−135.76 (4)	C25—P2—C19—C24	17.1 (3)
S4—W—S2—Ag3	137.82 (4)	C31—P2—C19—C20	84.3 (3)
S1—Ag2—S2—W	14.80 (3)	C31—P2—C19—C24	−94.1 (3)
S1—Ag2—S2—Ag3	93.26 (3)	P2—C19—C20—C21	−178.2 (3)
I—Ag2—S2—W	−85.33 (3)	C24—C19—C20—C21	0.2 (5)
I—Ag2—S2—Ag3	−6.87 (2)	C19—C20—C21—C22	0.5 (6)
P2—Ag2—S2—W	153.28 (4)	C20—C21—C22—C23	−0.7 (6)
P2—Ag2—S2—Ag3	−128.27 (4)	C21—C22—C23—C24	0.2 (6)
S3—Ag3—S2—W	−15.35 (3)	P2—C19—C24—C23	177.7 (3)
S3—Ag3—S2—Ag2	−92.29 (3)	C20—C19—C24—C23	−0.7 (6)
I—Ag3—S2—W	83.94 (3)	C22—C23—C24—C19	0.5 (6)
I—Ag3—S2—Ag2	7.00 (2)	Ag2—P2—C25—C26	−37.4 (3)
P3—Ag3—S2—W	−148.00 (3)	Ag2—P2—C25—C30	145.3 (3)
P3—Ag3—S2—Ag2	135.06 (4)	C19—P2—C25—C26	87.2 (3)
S1—W—S3—Ag1	14.20 (3)	C19—P2—C25—C30	−90.1 (3)
S1—W—S3—Ag3	104.73 (3)	C31—P2—C25—C26	−163.3 (3)
S2—W—S3—Ag1	−109.70 (3)	C31—P2—C25—C30	19.4 (4)
S2—W—S3—Ag3	−19.17 (4)	P2—C25—C26—C27	−176.4 (3)
S4—W—S3—Ag1	132.53 (3)	C30—C25—C26—C27	1.0 (6)
S4—W—S3—Ag3	−136.94 (3)	C25—C26—C27—C28	−0.4 (6)
S1—Ag1—S3—W	−11.82 (3)	C26—C27—C28—C29	−0.8 (6)
S1—Ag1—S3—Ag3	−88.52 (3)	C27—C28—C29—C30	1.4 (6)
I—Ag1—S3—W	88.76 (3)	P2—C25—C30—C29	176.9 (3)
I—Ag1—S3—Ag3	12.06 (2)	C26—C25—C30—C29	−0.4 (6)
P1—Ag1—S3—W	−156.29 (3)	C28—C29—C30—C25	−0.8 (6)

P1—Ag1—S3—Ag3	127.02 (4)	Ag2—P2—C31—C32	153.2 (3)
S2—Ag3—S3—W	15.43 (3)	Ag2—P2—C31—C36	−24.9 (3)
S2—Ag3—S3—Ag1	91.89 (3)	C19—P2—C31—C32	28.6 (3)
I—Ag3—S3—W	−88.69 (2)	C19—P2—C31—C36	−149.5 (3)
I—Ag3—S3—Ag1	−12.24 (2)	C25—P2—C31—C32	−80.6 (3)
P3—Ag3—S3—W	151.06 (3)	C25—P2—C31—C36	101.2 (3)
P3—Ag3—S3—Ag1	−132.48 (3)	P2—C31—C32—C33	−180.0 (3)
S2—Ag3—I—Ag1	−81.71 (3)	C36—C31—C32—C33	−1.8 (5)
S2—Ag3—I—Ag2	−6.25 (2)	C31—C32—C33—C34	0.8 (6)
S3—Ag3—I—Ag1	10.72 (2)	C32—C33—C34—C35	0.4 (6)
S3—Ag3—I—Ag2	86.19 (2)	C33—C34—C35—C36	−0.6 (6)
P3—Ag3—I—Ag1	140.24 (3)	P2—C31—C36—C35	179.9 (3)
P3—Ag3—I—Ag2	−144.30 (3)	C32—C31—C36—C35	1.7 (5)
S1—Ag2—I—Ag1	−10.84 (2)	C34—C35—C36—C31	−0.5 (6)
S1—Ag2—I—Ag3	−88.71 (2)	S2—Ag3—P3—C37	−81.18 (13)
S2—Ag2—I—Ag1	84.15 (2)	S2—Ag3—P3—C43	37.35 (14)
S2—Ag2—I—Ag3	6.27 (2)	S2—Ag3—P3—C49	157.96 (13)
P2—Ag2—I—Ag1	−139.79 (3)	S3—Ag3—P3—C37	159.75 (13)
P2—Ag2—I—Ag3	142.33 (3)	S3—Ag3—P3—C43	−81.72 (13)
S1—Ag1—I—Ag2	10.99 (2)	S3—Ag3—P3—C49	38.89 (13)
S1—Ag1—I—Ag3	84.07 (2)	I—Ag3—P3—C37	44.64 (13)
S3—Ag1—I—Ag2	−84.09 (2)	I—Ag3—P3—C43	163.17 (13)
S3—Ag1—I—Ag3	−11.00 (2)	I—Ag3—P3—C49	−76.23 (13)
P1—Ag1—I—Ag2	144.30 (3)	Ag3—P3—C37—C38	−36.4 (4)
P1—Ag1—I—Ag3	−142.62 (3)	Ag3—P3—C37—C42	144.7 (3)
S1—Ag1—P1—C1	51.69 (14)	C43—P3—C37—C38	−160.6 (3)
S1—Ag1—P1—C7	−68.66 (14)	C43—P3—C37—C42	20.4 (4)
S1—Ag1—P1—C13	170.85 (12)	C49—P3—C37—C38	88.6 (3)
S3—Ag1—P1—C1	−175.74 (13)	C49—P3—C37—C42	−90.4 (4)
S3—Ag1—P1—C7	63.92 (14)	P3—C37—C38—C39	−177.8 (3)
S3—Ag1—P1—C13	−56.57 (13)	C42—C37—C38—C39	1.2 (6)
I—Ag1—P1—C1	−62.83 (13)	C37—C38—C39—C40	0.1 (7)
I—Ag1—P1—C7	176.82 (13)	C38—C39—C40—C41	−1.0 (7)
I—Ag1—P1—C13	56.33 (12)	C39—C40—C41—C42	0.6 (7)
Ag1—P1—C1—C2	41.8 (3)	P3—C37—C42—C41	177.4 (4)
Ag1—P1—C1—C6	−141.1 (3)	C38—C37—C42—C41	−1.6 (7)
C7—P1—C1—C2	166.8 (3)	C40—C41—C42—C37	0.7 (7)
C7—P1—C1—C6	−16.1 (4)	Ag3—P3—C43—C44	−39.6 (3)
C13—P1—C1—C2	−82.3 (3)	Ag3—P3—C43—C48	142.8 (3)
C13—P1—C1—C6	94.8 (3)	C37—P3—C43—C44	87.2 (3)
P1—C1—C2—C3	176.9 (3)	C37—P3—C43—C48	−90.4 (3)
C6—C1—C2—C3	−0.4 (6)	C49—P3—C43—C44	−163.5 (3)
C1—C2—C3—C4	1.0 (6)	C49—P3—C43—C48	18.9 (3)
C2—C3—C4—C5	−0.8 (6)	P3—C43—C44—C45	−176.1 (3)
C3—C4—C5—C6	0.0 (6)	C48—C43—C44—C45	1.7 (6)
P1—C1—C6—C5	−177.6 (3)	C43—C44—C45—C46	−0.8 (6)
C2—C1—C6—C5	−0.5 (6)	C44—C45—C46—C47	−0.5 (7)
C4—C5—C6—C1	0.6 (6)	C45—C46—C47—C48	1.0 (7)
Ag1—P1—C7—C8	46.9 (3)	C46—C47—C48—C43	−0.1 (7)

Ag1—P1—C7—C12	−132.4 (3)	P3—C43—C48—C47	176.4 (3)
C1—P1—C7—C8	−80.1 (3)	C44—C43—C48—C47	−1.2 (6)
C1—P1—C7—C12	100.6 (3)	Ag3—P3—C49—C50	−24.5 (3)
C13—P1—C7—C8	171.0 (3)	Ag3—P3—C49—C54	155.5 (3)
C13—P1—C7—C12	−8.3 (4)	C37—P3—C49—C50	−152.3 (3)
P1—C7—C8—C9	177.4 (3)	C37—P3—C49—C54	27.6 (4)
C12—C7—C8—C9	−3.2 (6)	C43—P3—C49—C50	99.9 (3)
C7—C8—C9—C10	1.7 (7)	C43—P3—C49—C54	−80.1 (3)
C8—C9—C10—C11	0.9 (7)	P3—C49—C50—C51	179.9 (3)
C9—C10—C11—C12	−2.0 (7)	C54—C49—C50—C51	0.0 (6)
P1—C7—C12—C11	−178.6 (3)	C49—C50—C51—C52	−0.4 (6)
C8—C7—C12—C11	2.0 (6)	C50—C51—C52—C53	1.0 (6)
C10—C11—C12—C7	0.5 (6)	C51—C52—C53—C54	−1.2 (6)
Ag1—P1—C13—C14	−168.3 (2)	C52—C53—C54—C49	0.8 (6)
Ag1—P1—C13—C18	11.9 (3)	P3—C49—C54—C53	179.9 (3)
C1—P1—C13—C14	−42.0 (3)	C50—C49—C54—C53	−0.2 (6)
C1—P1—C13—C18	138.2 (3)	$C55^{i}$—Cl—C55—Cl^{i}	0.0

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

Fig. 1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