



Crystal structure of the unusual coordination polymer *catena*-poly[[gold(I)- μ -1,2-bis(diphenylphosphinothioyl)ethane- κ^2 S:S'] dibromidoaurate(I)]¹

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Keywords: crystal structure; polymer; phosphine sulfide; gold.

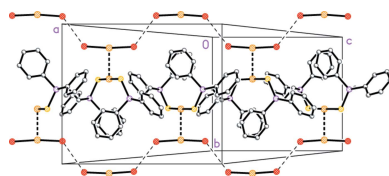
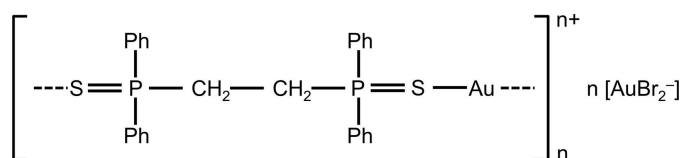
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In the title compound, $\{[\text{Au}(\text{C}_{26}\text{H}_{24}\text{P}_2\text{S}_2)][\text{AuBr}_2]\}_n$, the gold(I) centres of the cation are coordinated by the P=S groups of the disulfide ligands to form a chain polymer parallel to the *c* axis. Both independent gold atoms lie on the same twofold axis, and the midpoint of the H₂C–CH₂ bond lies on an inversion centre. The anions flank the polymeric chain; they are connected to it by short aurophilic interactions and C–H···Br contacts, and to each other by Br···Br contacts.

1. Chemical context

Although phosphane sulfides are known to act as ligands towards gold(I) centres, not many complexes have been structurally characterized in which two such ligands coordinate to gold(I). A search of the Cambridge Database (2019 Version, *ConQuest* 2.0.5) revealed only three structures involving the cation $[(\text{Ph}_3\text{P}=\text{S})_2\text{Au}]^+$; the PO₂F₂[−] salt (LeBlank *et al.*, 1997), the nitrate (Jones & Geissler, 2016*a*) and a bis(methylsulfonyl)amide salt (Jones & Geissler, 2016*b*). Cationic 1:1 complexes of gold(I) with diphosphane disulfides can only be achieved if the ligand geometry allows for linear coordination at the gold atom, which is not generally the case unless suitable spacers, such as ferrocene units or other metal centres, are present (Gimeno *et al.*, 2000, and references therein; Parkanyi & Besenyei, 2017; Wang & Fackler, 1990).



In the course of our studies of phosphane chalcogenide complexes of gold (Upmann *et al.*, 2019, and references therein) we planned to study complexes of the diphosphane disulfides 1,2-bis(diphenylphosphinothioyl)ethane [previously known as 1,2-bis(diphenylphosphino)ethane disulfide; dppeS₂] and bis(diphenylthiophosphinoyl)methane [previously known as bis(diphenylphosphino)methane disulfide; dppmS₂] with gold(I) halide fragments AuBr and AuCl, with particular attention to the mononuclear complexes. This succeeded to some extent; we were able to isolate and determine the structure of dppmS₂AuCl, the isotypic dppmS₂AuBr and its oxidation product with bromine $[(\text{dppmS}_2)\text{AuBr}_2]^+ [\text{AuBr}_4]^-$ (Jones *et al.*, 2020*a,b,c*, respectively), but yields were

Table 1
 Selected geometric parameters (Å, °).

Au1—S1	2.3125 (9)	Br1···Br1 ⁱ	3.7424 (8)
Au1···Au2	2.9622 (3)	P1—S1	2.0097 (12)
Au2—Br1	2.3746 (5)	C1—C1 ⁱⁱ	1.528 (6)
S1—Au1—S1 ⁱⁱⁱ	178.43 (4)	Br1—Au2···Au1	93.201 (11)
S1—Au1···Au2	90.78 (2)	Au2—Br1···Br1 ⁱ	126.21 (2)
Br1—Au2—Br1 ⁱⁱⁱ	173.60 (2)	P1—S1—Au1	98.34 (4)

Symmetry codes: (i) $-x + 1, -y + 2, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 1, y, -z + \frac{1}{2}$.

poor and it was clear that scrambling reactions were a problem. With dppeS₂ even less was achieved, but a few thin needles, isolated from the attempted synthesis of dppeS₂AuBr, proved to be an unusual coordination polymer [(dppeS₂)Au]²⁺_n·n[AuBr₂]⁻, the structure of which we report here.

2. Structural commentary

The title compound is shown in Fig. 1. The cation has the stoichiometry [dppeS₂Au]⁺, and forms a chain polymer (\cdots Au—S=PCH₂CH₂P=S \cdots)_n parallel to the *c* axis; the anion is [AuBr₂]⁻. Both gold atoms lie on twofold axes $\frac{1}{2}y, \frac{1}{4}z$ and show the linear coordination geometry expected for Au^I; the midpoint of the central H₂C—CH₂ bond lies on the inversion centre $\frac{1}{2}x, \frac{1}{2}y, \frac{1}{2}z$. Bond lengths and angles may be considered normal; for a selection, see Table 1. Coordination polymers are scarce for diphosphane disulfide ligands (see below).

3. Supramolecular features

The gold atoms of the cation and anion are connected *via* a short aurophilic contact of 2.9622 (3) Å, and the anions thus flank the cation polymer (Fig. 2). Neighbouring anions are connected by short Br···Br contacts of 3.7424 (8) Å (operator 1 - *x*, 2 - *y*, 1 - *z*), and also provide links to adjacent polymers (not shown in Fig. 2). We have previously noted an example of short contacts between dibromoaurate(I) anions

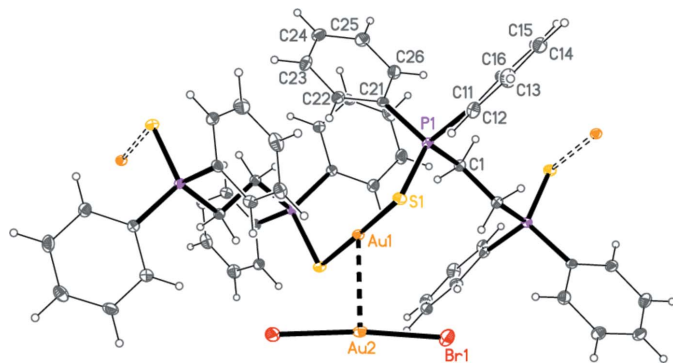


Figure 1
 Structure of the title complex in the crystal; the asymmetric unit is numbered. The aurophilic contact and the S—Au connections to the next gold atoms in the polymer are indicated by filled and open dashed bonds, respectively.

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C16—H16···Br1 ⁱⁱ	0.95	2.81	3.712 (4)	159
C26—H26···Br1 ⁱⁱ	0.95	2.89	3.775 (4)	155

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

(Döring & Jones, 2013); for a further example, see Beno *et al.* (1990). We have also described Br···Br and Cl···Cl contacts in a series of tetrabromidoaurate(III) and tetrachloridoaurate(III) salts (Döring & Jones, 2016).

Two C—H···Br contacts between cation and anions are sufficiently short and linear to be considered ‘weak’ hydrogen bonds (Table 2), and thus to contribute further cohesion to the structure, but are omitted from Fig. 2 for clarity.

4. Database survey

A database search (CSD 2019 Version, *ConQuest* 2.0.5) found 11 hits for systems involving two P=S units bonded to Au^I. The P=S bond lengths range from 1.985–2.039, av. 2.018 Å, and the S—Au bond lengths from 2.275–2.317, av. 2.296 Å. The only other coordination polymer found for a diphosphane disulfide was [(CuCN)₂(dppeS₂)]_n (Zhou *et al.*, 2006), a two-dimensional polymer involving four-coordinate Cu centres.

5. Synthesis and crystallization

The compound arose from an attempt to synthesize dppeS₂AuBr. A solution of thtAuBr (tht = tetrahydrothiophene; 0.775 g, 2.12 mmol) in CH₂Cl₂ (50 ml) was added to dppeS₂ (0.981 g, 2.12 mmol) dissolved in CH₂Cl₂ (50 ml). After stirring for 1 h, the solvent was removed, and the solid thus obtained was dried under vacuum and recrystallized from dichloromethane/*n*-pentane. The elemental analysis was approximately correct for the expected stoichiometry: calculated, C 42.23%, H 3.27%, S 8.67%; found, C 43.22%, H 3.87%, S 8.19%. However, attempts to obtain crystals suitable for X-ray structure analysis (by evaporation from a solution in CH₂Cl₂) led only to a few very thin needles of the title compound, with overall stoichiometry dppeS₂(AuBr)₂.

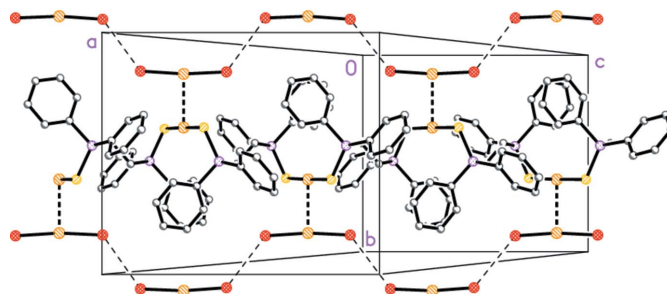


Figure 2
 The polymeric structure of the title compound, viewed perpendicular to the (101) plane. Aurophilic contacts are shown as thick bonds and Br···Br contacts as thin dashed bonds. Hydrogen atoms are omitted for clarity.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were included using a riding model starting from calculated positions ($C-H_{\text{aromatic}} = 0.95$, $C-H_{\text{methylene}} = 0.99 \text{ \AA}$). The $U_{\text{iso}}(\text{H})$ values were fixed at 1.2 times the equivalent U_{iso} value of the parent carbon atoms.

Acknowledgements

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Table 3

Experimental details.

Crystal data	
Chemical formula	[Au(C ₂₆ H ₂₄ P ₂ S ₂)] [AuBr ₂]
M_r	1016.26
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	100
a, b, c (Å)	21.4112 (8), 11.9708 (2), 13.7726 (4)
β (°)	128.316 (7)
V (Å ³)	2769.7 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	25.63
Crystal size (mm)	0.12 × 0.005 × 0.005
Data collection	
Diffraction	Oxford Diffraction Xcalibur, Atlas, Nova
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2010)
$T_{\text{min}}, T_{\text{max}}$	0.387, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27632, 2873, 2630
R_{int}	0.037
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.629
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.021, 0.053, 1.06
No. of reflections	2873
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.42, -0.99

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015) and *XP* (Siemens, 1994).

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Acta Cryst. (2020). E76, 1768-1770 [https://doi.org/10.1107/S2056989020013675]

Crystal structure of the unusual coordination polymer *catena*-poly[[gold(I)- μ -1,2-bis(diphenylphosphinothioyl)ethane- κ^2 S:S'] dibromidoaurate(I)]

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL2018/3* (Sheldrick, 2015).

catena-Poly[[gold(I)- μ -1,2-bis(diphenylphosphinothioyl)ethane- κ^2 S:S'] dibromidoaurate(I)]

Crystal data

[Au(C₂₆H₂₄P₂S₂)] [AuBr₂]

$M_r = 1016.26$

Monoclinic, *C2/c*

$a = 21.4112$ (8) Å

$b = 11.9708$ (2) Å

$c = 13.7726$ (4) Å

$\beta = 128.316$ (7)°

$V = 2769.7$ (3) Å³

$Z = 4$

$F(000) = 1880$

$D_x = 2.437$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 17272 reflections

$\theta = 4.1$ – 75.8 °

$\mu = 25.63$ mm⁻¹

$T = 100$ K

Needle, colourless

$0.12 \times 0.01 \times 0.01$ mm

Data collection

Oxford Diffraction Xcalibur, Atlas, Nova diffractometer

Radiation source: Nova (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.3543 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlisPro*; Oxford Diffraction, 2010)

$T_{\min} = 0.387$, $T_{\max} = 1.000$

27632 measured reflections

2873 independent reflections

2630 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 76.0$ °, $\theta_{\min} = 4.5$ °

$h = -26 \rightarrow 26$

$k = -14 \rightarrow 15$

$l = -17 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.053$

$S = 1.06$

2873 reflections

155 parameters

0 restraints

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

$$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 12.9976P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.42 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.99 \text{ e } \text{\AA}^{-3}$$

Special details

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

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Au1	0.500000	0.61954 (2)	0.250000	0.01687 (7)
Au2	0.500000	0.86699 (2)	0.250000	0.01950 (7)
Br1	0.47685 (3)	0.87807 (3)	0.39751 (4)	0.03124 (11)
P1	0.60133 (5)	0.46450 (7)	0.49985 (8)	0.01384 (16)
S1	0.61453 (5)	0.61690 (7)	0.45351 (8)	0.01915 (17)
C1	0.50616 (19)	0.4520 (3)	0.4701 (3)	0.0162 (7)
H1A	0.462644	0.452353	0.379701	0.019*
H1B	0.504140	0.380043	0.503474	0.019*
C11	0.6769 (2)	0.4432 (3)	0.6634 (3)	0.0167 (7)
C12	0.7460 (2)	0.5083 (3)	0.7329 (4)	0.0214 (8)
H12	0.752518	0.568996	0.695455	0.026*
C13	0.8047 (2)	0.4839 (4)	0.8566 (4)	0.0290 (9)
H13	0.851649	0.528125	0.903677	0.035*
C14	0.7962 (2)	0.3962 (4)	0.9128 (4)	0.0267 (8)
H14	0.836922	0.380547	0.997887	0.032*
C15	0.7280 (2)	0.3310 (3)	0.8446 (3)	0.0227 (7)
H15	0.721865	0.270674	0.882930	0.027*
C16	0.6684 (2)	0.3542 (3)	0.7197 (3)	0.0198 (7)
H16	0.621780	0.309224	0.672798	0.024*
C21	0.61000 (19)	0.3529 (3)	0.4211 (3)	0.0154 (6)
C22	0.6509 (2)	0.3700 (3)	0.3737 (4)	0.0220 (7)
H22	0.670919	0.441911	0.377148	0.026*
C23	0.6622 (3)	0.2805 (4)	0.3212 (4)	0.0287 (8)
H23	0.689530	0.291899	0.287999	0.034*
C24	0.6338 (2)	0.1754 (3)	0.3171 (4)	0.0274 (8)
H24	0.641465	0.114817	0.280842	0.033*
C25	0.5943 (2)	0.1586 (3)	0.3657 (4)	0.0264 (8)
H25	0.575405	0.086098	0.363559	0.032*
C26	0.5819 (3)	0.2461 (3)	0.4176 (4)	0.0237 (8)
H26	0.554451	0.233937	0.450538	0.028*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01921 (11)	0.01291 (10)	0.01950 (11)	0.000	0.01250 (9)	0.000
Au2	0.01812 (11)	0.01358 (10)	0.02586 (12)	0.000	0.01316 (9)	0.000

Br1	0.0371 (2)	0.0274 (2)	0.0408 (3)	-0.00694 (16)	0.0299 (2)	-0.00832 (17)
P1	0.0127 (4)	0.0131 (4)	0.0155 (4)	-0.0004 (3)	0.0086 (3)	-0.0009 (3)
S1	0.0192 (4)	0.0151 (4)	0.0211 (4)	-0.0024 (3)	0.0115 (4)	-0.0003 (3)
C1	0.0129 (15)	0.0177 (16)	0.0170 (16)	-0.0012 (12)	0.0088 (13)	-0.0015 (13)
C11	0.0153 (15)	0.0178 (16)	0.0192 (17)	0.0005 (12)	0.0117 (14)	-0.0041 (13)
C12	0.0180 (17)	0.0258 (19)	0.0236 (19)	-0.0060 (14)	0.0144 (16)	-0.0051 (15)
C13	0.0168 (17)	0.041 (2)	0.022 (2)	-0.0063 (16)	0.0087 (16)	-0.0067 (17)
C14	0.0164 (17)	0.040 (2)	0.0161 (18)	0.0064 (15)	0.0063 (15)	-0.0014 (16)
C15	0.0236 (18)	0.0245 (18)	0.0183 (18)	0.0060 (14)	0.0121 (15)	0.0027 (14)
C16	0.0170 (16)	0.0182 (16)	0.0197 (18)	0.0009 (13)	0.0091 (14)	-0.0008 (13)
C21	0.0139 (15)	0.0147 (15)	0.0160 (16)	0.0032 (12)	0.0085 (14)	0.0022 (12)
C22	0.0235 (18)	0.0204 (17)	0.0269 (19)	0.0039 (13)	0.0181 (16)	0.0025 (14)
C23	0.033 (2)	0.032 (2)	0.035 (2)	0.0043 (17)	0.0276 (19)	0.0005 (18)
C24	0.032 (2)	0.0236 (19)	0.026 (2)	0.0078 (16)	0.0173 (17)	-0.0010 (15)
C25	0.034 (2)	0.0164 (17)	0.028 (2)	-0.0033 (15)	0.0186 (18)	-0.0053 (15)
C26	0.028 (2)	0.0203 (19)	0.026 (2)	-0.0037 (13)	0.0187 (18)	-0.0027 (14)

Geometric parameters (Å, °)

Au1—S1	2.3125 (9)	C13—H13	0.9500
Au1—S1 ⁱ	2.3125 (9)	C14—C15	1.387 (6)
Au1—Au2	2.9622 (3)	C14—H14	0.9500
Au2—Br1	2.3746 (5)	C15—C16	1.393 (5)
Au2—Br1 ⁱ	2.3746 (5)	C15—H15	0.9500
Br1—Br1 ⁱⁱ	3.7424 (8)	C16—H16	0.9500
P1—C11	1.800 (4)	C21—C22	1.394 (5)
P1—C21	1.801 (4)	C21—C26	1.401 (5)
P1—C1	1.819 (3)	C22—C23	1.394 (5)
P1—S1	2.0097 (12)	C22—H22	0.9500
C1—C1 ⁱⁱⁱ	1.528 (6)	C23—C24	1.384 (6)
C1—H1A	0.9900	C23—H23	0.9500
C1—H1B	0.9900	C24—C25	1.381 (6)
C11—C16	1.395 (5)	C24—H24	0.9500
C11—C12	1.399 (5)	C25—C26	1.384 (5)
C12—C13	1.382 (6)	C25—H25	0.9500
C12—H12	0.9500	C26—H26	0.9500
C13—C14	1.383 (6)		
S1—Au1—S1 ⁱ	178.43 (4)	C14—C13—H13	119.5
S1—Au1—Au2	90.78 (2)	C13—C14—C15	119.9 (4)
S1 ⁱ —Au1—Au2	90.78 (2)	C13—C14—H14	120.1
Br1—Au2—Br1 ⁱ	173.60 (2)	C15—C14—H14	120.1
Br1—Au2—Au1	93.201 (11)	C14—C15—C16	119.9 (4)
Br1 ⁱ —Au2—Au1	93.201 (11)	C14—C15—H15	120.1
Au2—Br1—Br1 ⁱⁱ	126.21 (2)	C16—C15—H15	120.1
C11—P1—C21	107.45 (15)	C15—C16—C11	120.2 (3)
C11—P1—C1	106.44 (16)	C15—C16—H16	119.9
C21—P1—C1	108.84 (15)	C11—C16—H16	119.9

C11—P1—S1	109.38 (12)	C22—C21—C26	119.9 (3)
C21—P1—S1	113.24 (12)	C22—C21—P1	120.2 (3)
C1—P1—S1	111.20 (12)	C26—C21—P1	119.7 (3)
P1—S1—Au1	98.34 (4)	C21—C22—C23	119.4 (4)
C1 ⁱⁱⁱ —C1—P1	111.1 (3)	C21—C22—H22	120.3
C1 ⁱⁱⁱ —C1—H1A	109.4	C23—C22—H22	120.3
P1—C1—H1A	109.4	C24—C23—C22	120.5 (4)
C1 ⁱⁱⁱ —C1—H1B	109.4	C24—C23—H23	119.8
P1—C1—H1B	109.4	C22—C23—H23	119.8
H1A—C1—H1B	108.0	C25—C24—C23	119.8 (4)
C16—C11—C12	119.5 (3)	C25—C24—H24	120.1
C16—C11—P1	118.5 (3)	C23—C24—H24	120.1
C12—C11—P1	121.8 (3)	C24—C25—C26	120.8 (4)
C13—C12—C11	119.6 (4)	C24—C25—H25	119.6
C13—C12—H12	120.2	C26—C25—H25	119.6
C11—C12—H12	120.2	C25—C26—C21	119.5 (4)
C12—C13—C14	121.0 (4)	C25—C26—H26	120.2
C12—C13—H13	119.5	C21—C26—H26	120.2
S1—Au1—Au2—Br1	-65.75 (3)	C11—C12—C13—C14	-0.2 (6)
S1 ⁱ —Au1—Au2—Br1	114.25 (2)	C12—C13—C14—C15	0.2 (6)
S1—Au1—Au2—Br1 ⁱ	114.24 (3)	C13—C14—C15—C16	0.1 (6)
S1 ⁱ —Au1—Au2—Br1 ⁱ	-65.75 (3)	C14—C15—C16—C11	-0.4 (6)
Au1—Au2—Br1—Br1 ⁱⁱ	158.03 (3)	C12—C11—C16—C15	0.5 (5)
C11—P1—S1—Au1	-172.78 (12)	P1—C11—C16—C15	176.2 (3)
C21—P1—S1—Au1	67.42 (12)	C11—P1—C21—C22	-98.2 (3)
C1—P1—S1—Au1	-55.51 (12)	C1—P1—C21—C22	146.9 (3)
Au2—Au1—S1—P1	156.28 (4)	S1—P1—C21—C22	22.7 (3)
C11—P1—C1—C1 ⁱⁱⁱ	67.1 (4)	C11—P1—C21—C26	76.0 (3)
C21—P1—C1—C1 ⁱⁱⁱ	-177.3 (3)	C1—P1—C21—C26	-38.9 (3)
S1—P1—C1—C1 ⁱⁱⁱ	-51.9 (4)	S1—P1—C21—C26	-163.1 (3)
C21—P1—C11—C16	-70.7 (3)	C26—C21—C22—C23	1.1 (6)
C1—P1—C11—C16	45.7 (3)	P1—C21—C22—C23	175.3 (3)
S1—P1—C11—C16	166.0 (2)	C21—C22—C23—C24	-0.6 (6)
C21—P1—C11—C12	104.9 (3)	C22—C23—C24—C25	-0.3 (6)
C1—P1—C11—C12	-138.7 (3)	C23—C24—C25—C26	0.7 (6)
S1—P1—C11—C12	-18.4 (3)	C24—C25—C26—C21	-0.2 (6)
C16—C11—C12—C13	-0.2 (5)	C22—C21—C26—C25	-0.7 (6)
P1—C11—C12—C13	-175.7 (3)	P1—C21—C26—C25	-174.9 (3)

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

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16 \cdots Br1 ⁱⁱⁱ	0.95	2.81	3.712 (4)	159
C26—H26 \cdots Br1 ⁱⁱⁱ	0.95	2.89	3.775 (4)	155

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