Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[bis(dicyclohexylphosphino)ethane-κ^2P,P']-gold(I) chloride chloroform tetrasolvate

William Clegg,[a]* Andrew J. Scott,[a] Christian Wiesauer,[b]‡ Walter Weissensteiner[b] and Todd B. Marder[c]‡

[a]School of Natural Sciences (Chemistry), University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, England, [b]Institute of Organic Chemistry, University of Vienna, Waehringerstrasse 38, A-1090 Wien, Austria, and [c]Department of Chemistry, University of Durham, Durham DH1 3LE, England

‡ Formerly at Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

Correspondence e-mail: w.clegg@ncl.ac.uk

Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.018 Å
Disorder in main residue
R factor = 0.082
wR factor = 0.223
Data-to-parameter ratio = 17.2

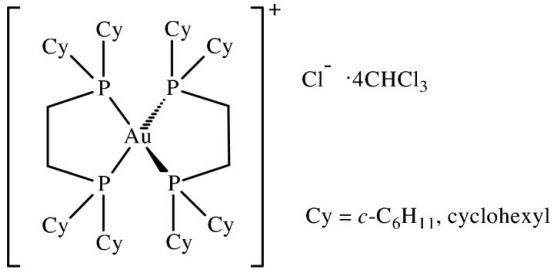
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 June 2004
Accepted 11 June 2004
Online 19 June 2004

In the title complex, $[Au(C_{26}H_{48}P_2)_2]Cl\cdot4CHCl_3$, the cation and anion lie on twofold rotation axes. The Au atom has a distorted tetrahedral coordination geometry, with two chelating diphosphine ligands, and lies far from the anion.

Comment

As part of a study of hydroboration catalysis, the title compound, (I), was prepared as a catalyst precursor. Although gold complexes with the ligands DCPE [bis(dicyclohexylphosphino)ethane] and DPPB [bis(diphenylphosphino)butane] are effective alkene diboration catalysts (Baker *et al.*, 1995), we found them to be ineffective for hydroboration of vinylboronate esters.



(I)

The crystal structure of the chloroform tetrasolvate has been determined. The complex consists of a bis(diphosphine)gold(I) cation, a chloride anion and four molecules of chloroform. The cation and anion lie on twofold rotation axes in space group $C2/c$ and the asymmetric unit contains two solvent molecules, one of which is disordered.

The Au atom is coordinated by two chelating diphosphine ligands in a distorted tetrahedral geometry (Fig. 1 and Table 1), the main distortion being the small bite angles of the ligands. A similar geometry is found for nine other gold(I) complexes of diphosphinoethane ligands in the Cambridge Structural Database (CSD, Version 5.25 with one update, January 2004; Allen, 2002), and is as expected. The CSD contains 103 structures of complexes of the DCPE ligand (the structure of the uncomplexed ligand has not been reported); almost all of these are with metals of the Fe/Ru/Os, Co/Rh/Ir and (especially) Ni/Pd/Pt transition-metal triads. There are two complexes with Cu, one with Al, and three with Au. In the vast majority of complexes, DCPE coordinates as a chelating ligand, and there are six incidences of DCPE as a bridging ligand, including all of the previously reported gold complexes. In $[(DCPE)_2Au_2](PF_6)_2$, two DCPE ligands bridge a pair of Au^I atoms with a direct Au—Au bond (Schaefer *et al.*,

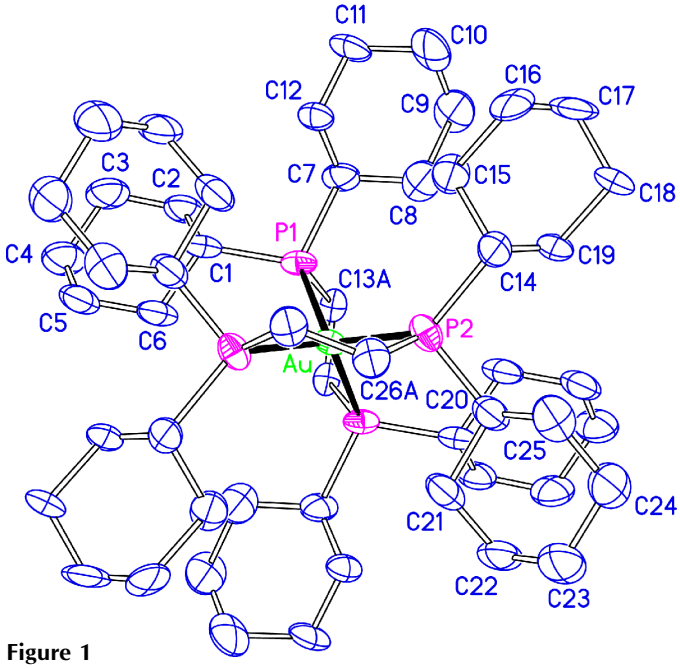


Figure 1
The structure of the cation of (I), shown with atom labels and 40% probability ellipsoids. H atoms and one of the disorder components have been omitted.

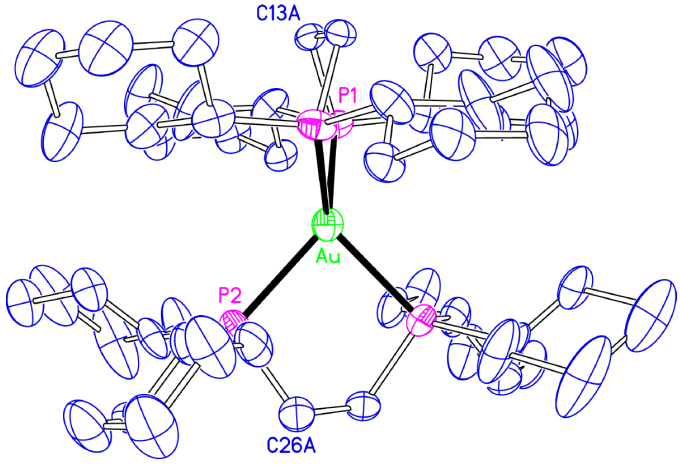


Figure 2
An alternative view of the cation, showing the conformation of the chelate rings.

1991). [BrAu(DCPE)AuCN] has a bridge between two well separated Au atoms (Schaefer *et al.*, 1992). $[(DCPE)_3Au_2][Au(CN)_2]_2$ contains one bridging and two chelating ligands (McCleskey *et al.*, 1993). Thus, there is considerably more variety in the coordination of DCPE to gold(I) than to other metals.

The ethylene linkages in the two DCPE ligands are disordered over two positions each, with staggered conformations, as indicated by P—C—C—P torsion angles of −50 (2), 47 (2), 52 (2) and −52 (2)° (two disorder components of two ligands). There is probably unresolved disorder also in the cyclohexyl groups.

The chloride anion has no significant non-Coulombic interactions and is >6.9 Å from the closest Au atoms. One of the two independent chloroform solvent molecules is disordered over two orientations by rotation about its C—H bond, while no disorder was resolved for the other solvent molecule.

Experimental

The title compound was prepared by the reaction of $Au(PEt_3)Cl$ with two equivalents of DCPE in THF solution. The reaction mixture was stirred for 5 h, then the solvent was removed *in vacuo*, leaving a fine white powder. This was recrystallized from chloroform. ^{1}HNMR (200 MHz): δ 1.28 (*s*, *br*, 22H), 1.85 (*s*, *br*, 22H). ^{31}P{^{1}H} NMR (81 MHz, CD_2Cl_2): δ 29.7.

Crystal data

$[Au(C_{26}H_{48}P_2)_2]Cl\cdot 4CHCl_3$	D_x = 1.379 Mg m^{-3}
M_r = 1555.06	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 13280 reflections
a = 25.939 (4) Å	θ = 1.7–27.8°
b = 13.938 (3) Å	μ = 2.55 mm^{-1}
c = 22.685 (4) Å	T = 160 (2) K
β = 114.050 (4)°	Plate, colourless
V = 7489 (2) Å^3	0.30 × 0.24 × 0.05 mm
Z = 4	

Data collection

Bruker SMART 1K CCD diffractometer	6599 independent reflections
	4771 reflections with $I > 2\sigma(I)$
Thin-slice ω scans	R_{int} = 0.077
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	θ_{max} = 25.0°
	$h = -30 \rightarrow 26$
T_{min} = 0.294, T_{max} = 0.881	$k = -16 \rightarrow 16$
19047 measured reflections	$l = -26 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1563P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.082	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.223	$\Delta\rho_{max}$ = 3.63 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −3.76 e Å^{-3}
6599 reflections	Extinction correction: *SHELXTL*
384 parameters	Extinction coefficient: 0.00045 (13)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Au—P1	2.434 (2)	Au—P2	2.470 (2)
P1—Au—P1^i	85.97 (11)	P1—Au—P2^i	113.49 (9)
P1—Au—P2	131.15 (9)	P2—Au—P2^i	87.53 (12)

Symmetry code: (i) $-x, y, \frac{1}{2}-z$.

H atoms were positioned geometrically and refined with a riding model, with C—H = 0.99–1.00 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Initial refinement produced highly anisotropic displacement parameters for the C atoms of the two ethylene linkages, which had apparently eclipsed arrangements. Each of these C atoms was successfully refined as two disorder components, the twofold rotation symmetry being retained for each component. Refined occupancy factors for the two linkages were 0.47:0.53 (2) and 0.52:0.48 (3). Twofold disorder was also resolved and refined for one of the chloroform molecules, with occupancies of 0.489:0.511 (9). Restraints were applied to geometry and displacement parameters in the disordered groups. The largest positive and negative features of the final difference map lie close to Au and to the disordered solvent molecule.

Data collection: *SMART* (Bruker, 2001); cell refinement: local programs; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; soft-

ware used to prepare material for publication: *SHELXTL* and local programs.

We thank the EPSRC (UK) and NSERC (Canada) for financial support. CW thanks the Austrian Ministry of Education, Science and Culture for supporting his stay at the University of Waterloo, Canada.

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supporting information

Acta Cryst. (2004). E**60**, m968–m970 [https://doi.org/10.1107/S1600536804014187]

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$V = 7489$ (2) Å^3
$Z = 4$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13280 reflections
$\theta = 1.7$–27.8°
$\mu = 2.55$ mm^{-1}
$T = 160$ K
Block, colourless
0.30 × 0.24 × 0.05 mm

Data collection

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Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
thin–slice ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1997)
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19047 measured reflections
6599 independent reflections
4771 reflections with $I > 2\sigma(I)$
$R_{int} = 0.077$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -30 \rightarrow 26$
$k = -16 \rightarrow 16$
$l = -26 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.082$
$wR(F^2) = 0.223$
$S = 1.01$
6599 reflections
384 parameters
118 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1563P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 3.63$ e Å^{-3}
$\Delta\rho_{min} = -3.76$ e Å^{-3}
Extinction correction: SHELXTL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00045 (13)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Au	0.0000	0.31327 (3)	0.2500	0.0421 (3)	

P1	−0.00060 (12)	0.18549 (15)	0.17656 (12)	0.0440 (6)	
C1	−0.0696 (5)	0.1755 (7)	0.1014 (5)	0.051 (2)	
H1	−0.0706	0.2326	0.0743	0.062*	
C2	−0.0755 (5)	0.0875 (9)	0.0580 (5)	0.067 (3)	
H2A	−0.0760	0.0282	0.0818	0.081*	
H2B	−0.0427	0.0842	0.0463	0.081*	
C3	−0.1306 (6)	0.0946 (11)	−0.0040 (6)	0.083 (4)	
H3A	−0.1340	0.0373	−0.0311	0.099*	
H3B	−0.1286	0.1518	−0.0289	0.099*	
C4	−0.1847 (6)	0.1022 (11)	0.0109 (6)	0.089 (4)	
H4A	−0.2186	0.1100	−0.0300	0.107*	
H4B	−0.1891	0.0426	0.0321	0.107*	
C5	−0.1792 (5)	0.1888 (9)	0.0553 (6)	0.082 (4)	
H5A	−0.1802	0.2489	0.0317	0.099*	
H5B	−0.2115	0.1895	0.0680	0.099*	
C6	−0.1240 (5)	0.1837 (8)	0.1159 (6)	0.064 (3)	
H6A	−0.1255	0.1276	0.1419	0.077*	
H6B	−0.1208	0.2420	0.1422	0.077*	
C7	0.0577 (5)	0.1598 (8)	0.1469 (5)	0.060 (3)	
H7	0.0515	0.0934	0.1287	0.072*	
C8	0.1185 (6)	0.1628 (13)	0.2034 (7)	0.107 (6)	
H8A	0.1203	0.1171	0.2376	0.128*	
H8B	0.1260	0.2279	0.2225	0.128*	
C9	0.1659 (6)	0.1356 (14)	0.1780 (7)	0.105 (5)	
H9A	0.2037	0.1418	0.2139	0.126*	
H9B	0.1610	0.0680	0.1634	0.126*	
C10	0.1626 (6)	0.1994 (10)	0.1234 (8)	0.091 (5)	
H10A	0.1900	0.1774	0.1060	0.110*	
H10B	0.1726	0.2659	0.1393	0.110*	
C11	0.1018 (5)	0.1972 (8)	0.0689 (7)	0.068 (3)	
H11A	0.0935	0.1315	0.0510	0.082*	
H11B	0.1002	0.2407	0.0337	0.082*	
C12	0.0548 (4)	0.2284 (8)	0.0932 (5)	0.051 (2)	
H12A	0.0617	0.2951	0.1096	0.061*	
H12B	0.0170	0.2254	0.0571	0.061*	
C13A	0.0141 (9)	0.0705 (10)	0.2269 (8)	0.043 (3)	0.47 (2)
H13A	0.0006	0.0147	0.1976	0.051*	0.47 (2)
H13B	0.0554	0.0634	0.2516	0.051*	0.47 (2)
C13B	−0.0135 (7)	0.0688 (8)	0.2143 (5)	0.033 (3)	0.53 (2)
H13C	−0.0547	0.0595	0.2001	0.040*	0.53 (2)
H13D	0.0012	0.0139	0.1981	0.040*	0.53 (2)
P2	0.06951 (10)	0.44125 (18)	0.30248 (13)	0.0489 (6)	
C14	0.1390 (4)	0.4634 (8)	0.2931 (5)	0.059 (3)	
H14	0.1519	0.5296	0.3095	0.070*	
C15	0.1289 (5)	0.4616 (13)	0.2215 (6)	0.103 (6)	
H15A	0.1000	0.5096	0.1971	0.124*	
H15B	0.1154	0.3974	0.2029	0.124*	
C16	0.1880 (7)	0.4862 (16)	0.2171 (6)	0.138 (8)	

H16A	0.1825	0.4837	0.1713	0.166*	
H16B	0.1993	0.5523	0.2328	0.166*	
C17	0.2353 (6)	0.4172 (12)	0.2562 (6)	0.110 (6)	
H17A	0.2255	0.3515	0.2386	0.132*	
H17B	0.2707	0.4363	0.2525	0.132*	
C18	0.2444 (4)	0.4179 (9)	0.3253 (5)	0.068 (3)	
H18A	0.2588	0.4814	0.3446	0.082*	
H18B	0.2726	0.3686	0.3494	0.082*	
C19	0.1860 (4)	0.3962 (8)	0.3302 (5)	0.058 (3)	
H19A	0.1742	0.3301	0.3146	0.070*	
H19B	0.1922	0.3985	0.3762	0.070*	
C20	0.0932 (4)	0.4494 (8)	0.3901 (5)	0.060 (3)	
H20	0.1165	0.3907	0.4082	0.072*	
C21	0.0405 (4)	0.4426 (8)	0.4103 (6)	0.067 (3)	
H21A	0.0167	0.5007	0.3955	0.080*	
H21B	0.0171	0.3861	0.3894	0.080*	
C22	0.0618 (5)	0.4338 (10)	0.4827 (6)	0.093 (5)	
H22A	0.0836	0.3737	0.4971	0.112*	
H22B	0.0293	0.4310	0.4950	0.112*	
C23	0.0997 (6)	0.5203 (12)	0.5164 (8)	0.110 (6)	
H23A	0.1136	0.5125	0.5637	0.133*	
H23B	0.0769	0.5798	0.5042	0.133*	
C24	0.1517 (6)	0.5306 (11)	0.4975 (7)	0.092 (5)	
H24A	0.1734	0.5890	0.5177	0.110*	
H24B	0.1770	0.4744	0.5138	0.110*	
C25	0.1314 (5)	0.5368 (8)	0.4254 (6)	0.070 (3)	
H25A	0.1644	0.5394	0.4141	0.083*	
H25B	0.1097	0.5970	0.4101	0.083*	
C26A	0.0235 (7)	0.5539 (10)	0.2833 (7)	0.052 (5)	0.52 (3)
H26A	0.0069	0.5601	0.3154	0.063*	0.52 (3)
H26B	0.0477	0.6107	0.2876	0.063*	0.52 (3)
C26B	0.0312 (5)	0.5540 (11)	0.2583 (12)	0.051 (5)	0.48 (3)
H26C	0.0485	0.6106	0.2856	0.062*	0.48 (3)
H26D	0.0370	0.5607	0.2179	0.062*	0.48 (3)
Cl1	0.0000	0.8143 (2)	0.2500	0.0493 (8)	
C27	−0.1456 (5)	−0.1686 (8)	0.1437 (6)	0.068 (3)	
H27	−0.1048	−0.1675	0.1739	0.081*	
Cl2	−0.1774 (2)	−0.2661 (3)	0.1644 (3)	0.1325 (19)	
Cl3	−0.1499 (4)	−0.1800 (3)	0.0658 (2)	0.154 (3)	
Cl4	−0.17644 (17)	−0.0626 (2)	0.15392 (17)	0.0848 (10)	
C28	0.0570 (4)	0.2082 (6)	0.6405 (5)	0.085 (3)	
H28	0.0498	0.2164	0.6802	0.102*	
Cl5	0.1106 (5)	0.2996 (6)	0.6464 (4)	0.135 (5)	0.489 (9)
Cl6	−0.0023 (5)	0.2262 (15)	0.5816 (6)	0.216 (9)	0.489 (9)
Cl7	0.0923 (5)	0.1022 (5)	0.6504 (6)	0.133 (5)	0.489 (9)
Cl5X	0.0274 (4)	0.1082 (5)	0.5850 (4)	0.099 (3)	0.511 (9)
Cl6X	0.1247 (4)	0.2007 (10)	0.6789 (5)	0.168 (7)	0.511 (9)
Cl7X	0.0286 (6)	0.3084 (5)	0.5905 (4)	0.123 (4)	0.511 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au	0.0404 (3)	0.0480 (4)	0.0475 (3)	0.000	0.0279 (2)	0.000
P1	0.0601 (15)	0.0375 (13)	0.0483 (13)	0.0075 (10)	0.0364 (12)	0.0020 (10)
C1	0.064 (6)	0.054 (6)	0.058 (6)	−0.004 (5)	0.047 (5)	−0.007 (5)
C2	0.072 (7)	0.080 (8)	0.069 (7)	−0.005 (6)	0.048 (6)	−0.023 (6)
C3	0.097 (10)	0.103 (10)	0.065 (7)	−0.012 (8)	0.050 (7)	−0.028 (7)
C4	0.087 (9)	0.118 (11)	0.075 (8)	−0.032 (8)	0.046 (7)	−0.042 (8)
C5	0.056 (7)	0.132 (13)	0.076 (8)	−0.029 (6)	0.045 (6)	−0.041 (7)
C6	0.068 (7)	0.077 (8)	0.070 (7)	−0.017 (5)	0.052 (6)	−0.021 (6)
C7	0.068 (7)	0.068 (7)	0.058 (6)	0.026 (5)	0.041 (5)	0.004 (5)
C8	0.073 (9)	0.175 (15)	0.071 (8)	0.071 (9)	0.028 (7)	−0.007 (9)
C9	0.074 (9)	0.156 (14)	0.087 (10)	0.063 (10)	0.036 (8)	−0.012 (10)
C10	0.058 (8)	0.122 (12)	0.104 (11)	0.018 (7)	0.043 (7)	−0.034 (9)
C11	0.063 (7)	0.084 (9)	0.085 (8)	0.010 (5)	0.058 (7)	0.001 (6)
C12	0.054 (6)	0.053 (6)	0.057 (6)	0.008 (5)	0.035 (5)	0.000 (5)
C13A	0.043 (5)	0.031 (4)	0.045 (4)	0.005 (4)	0.009 (4)	−0.004 (3)
C13B	0.033 (5)	0.025 (4)	0.046 (4)	0.004 (4)	0.021 (4)	−0.008 (3)
P2	0.0383 (13)	0.0443 (14)	0.0645 (15)	−0.0072 (10)	0.0213 (11)	0.0016 (12)
C14	0.053 (6)	0.070 (7)	0.050 (5)	−0.033 (5)	0.019 (5)	0.005 (5)
C15	0.069 (8)	0.171 (15)	0.060 (7)	−0.060 (9)	0.017 (6)	0.036 (8)
C16	0.112 (12)	0.26 (2)	0.043 (6)	−0.108 (14)	0.031 (8)	0.020 (10)
C17	0.103 (11)	0.188 (17)	0.077 (9)	−0.072 (12)	0.076 (9)	−0.041 (10)
C18	0.052 (6)	0.102 (9)	0.072 (7)	−0.015 (6)	0.046 (5)	0.003 (6)
C19	0.053 (6)	0.080 (8)	0.053 (5)	−0.021 (5)	0.034 (5)	0.007 (5)
C20	0.046 (6)	0.072 (7)	0.071 (7)	−0.009 (5)	0.033 (5)	−0.012 (6)
C21	0.046 (6)	0.077 (8)	0.090 (8)	−0.014 (5)	0.040 (6)	−0.030 (6)
C22	0.075 (8)	0.143 (13)	0.086 (8)	−0.034 (8)	0.058 (7)	−0.062 (9)
C23	0.083 (10)	0.155 (15)	0.110 (11)	−0.023 (9)	0.057 (9)	−0.072 (11)
C24	0.074 (9)	0.108 (11)	0.096 (10)	−0.027 (8)	0.037 (7)	−0.056 (9)
C25	0.066 (7)	0.048 (6)	0.096 (9)	−0.005 (5)	0.034 (6)	−0.027 (6)
C26A	0.054 (8)	0.044 (6)	0.057 (12)	−0.002 (5)	0.020 (7)	0.020 (8)
C26B	0.050 (8)	0.047 (6)	0.061 (12)	−0.001 (5)	0.027 (7)	0.015 (8)
Cl1	0.0535 (19)	0.052 (2)	0.0602 (19)	0.000	0.0408 (16)	0.000
C27	0.062 (7)	0.093 (9)	0.054 (6)	−0.010 (6)	0.030 (5)	0.003 (6)
Cl2	0.141 (4)	0.079 (3)	0.238 (6)	−0.001 (2)	0.139 (4)	0.020 (3)
Cl3	0.298 (9)	0.107 (4)	0.088 (3)	0.040 (4)	0.110 (4)	0.000 (2)
Cl4	0.119 (3)	0.073 (2)	0.089 (2)	0.0016 (18)	0.069 (2)	−0.0029 (17)
C28	0.095 (7)	0.115 (7)	0.079 (7)	0.011 (5)	0.068 (6)	0.004 (6)
Cl5	0.257 (13)	0.086 (6)	0.092 (6)	−0.058 (6)	0.102 (7)	−0.009 (5)
Cl6	0.122 (8)	0.41 (3)	0.112 (9)	0.032 (10)	0.045 (6)	0.101 (13)
Cl7	0.196 (11)	0.068 (4)	0.224 (13)	−0.002 (5)	0.178 (11)	−0.001 (6)
Cl5X	0.161 (8)	0.069 (4)	0.097 (5)	−0.008 (4)	0.084 (5)	0.002 (4)
Cl6X	0.080 (5)	0.32 (2)	0.098 (7)	0.021 (7)	0.030 (5)	−0.027 (8)
Cl7X	0.220 (12)	0.062 (4)	0.094 (5)	−0.002 (5)	0.072 (7)	−0.002 (4)

Geometric parameters (Å, º)

Au—P1	2.434 (2)	C14—H14	1.000
Au—P1^{i}	2.434 (2)	C14—C15	1.536 (15)
Au—P2	2.470 (2)	C14—C19	1.496 (15)
Au—P2^{i}	2.470 (2)	C15—H15A	0.990
P1—C1	1.910 (12)	C15—H15B	0.990
P1—C7	1.922 (10)	C15—C16	1.613 (18)
P1—C13A	1.914 (13)	C16—H16A	0.990
P1—C13B	1.930 (12)	C16—H16B	0.990
C1—H1	1.000	C16—C17	1.53 (2)
C1—C2	1.541 (13)	C17—H17A	0.990
C1—C6	1.578 (14)	C17—H17B	0.990
C2—H2A	0.990	C17—C18	1.489 (15)
C2—H2B	0.990	C18—H18A	0.990
C2—C3	1.547 (17)	C18—H18B	0.990
C3—H3A	0.990	C18—C19	1.590 (12)
C3—H3B	0.990	C19—H19A	0.990
C3—C4	1.575 (17)	C19—H19B	0.990
C4—H4A	0.990	C20—H20	1.000
C4—H4B	0.990	C20—C21	1.612 (14)
C4—C5	1.541 (16)	C20—C25	1.569 (14)
C5—H5A	0.990	C21—H21A	0.990
C5—H5B	0.990	C21—H21B	0.990
C5—C6	1.530 (18)	C21—C22	1.509 (17)
C6—H6A	0.990	C22—H22A	0.990
C6—H6B	0.990	C22—H22B	0.990
C7—H7	1.000	C22—C23	1.546 (17)
C7—C8	1.577 (18)	C23—H23A	0.990
C7—C12	1.529 (15)	C23—H23B	0.990
C8—H8A	0.990	C23—C24	1.580 (19)
C8—H8B	0.990	C24—H24A	0.990
C8—C9	1.602 (18)	C24—H24B	0.990
C9—H9A	0.990	C24—C25	1.504 (19)
C9—H9B	0.990	C25—H25A	0.990
C9—C10	1.50 (2)	C25—H25B	0.990
C10—H10A	0.990	C26A—C26A^{i}	1.50 (2)
C10—H10B	0.990	C26A—H26A	0.990
C10—C11	1.558 (19)	C26A—H26B	0.990
C11—H11A	0.990	C26B—C26B^{i}	1.51 (2)
C11—H11B	0.990	C26B—H26C	0.990
C11—C12	1.588 (13)	C26B—H26D	0.990
C12—H12A	0.990	C27—H27	1.000
C12—H12B	0.990	C27—Cl2	1.749 (12)
C13A—C13A^{i}	1.50 (2)	C27—Cl3	1.733 (12)
C13A—H13A	0.990	C27—Cl4	1.741 (13)
C13A—H13B	0.990	C28—H28	1.000
C13B—C13B^{i}	1.48 (2)	C28—Cl5	1.849 (11)

C13B—H13C	0.990	C28—Cl6	1.593 (11)
C13B—H13D	0.990	C28—Cl7	1.704 (10)
P2—C14	1.924 (10)	C28—Cl5X	1.824 (11)
P2—C20	1.829 (11)	C28—Cl6X	1.615 (11)
P2—C26A	1.912 (14)	C28—Cl7X	1.760 (10)
P2—C26B	1.911 (14)		

P1—Au—P1^{i}	85.97 (11)	C14—P2—C26B	96.9 (6)
P1—Au—P2	131.15 (9)	C20—P2—C26A	95.7 (6)
P1^{i}—Au—P2	113.49 (9)	C20—P2—C26B	113.1 (9)
P1—Au—P2^{i}	113.49 (9)	P2—C14—H14	107.2
P1^{i}—Au—P2^{i}	131.15 (9)	P2—C14—C15	110.5 (7)
P2—Au—P2^{i}	87.53 (12)	P2—C14—C19	115.0 (6)
Au—P1—C1	114.0 (3)	H14—C14—C15	107.2
Au—P1—C7	126.1 (4)	H14—C14—C19	107.2
Au—P1—C13A	105.1 (4)	C15—C14—C19	109.4 (11)
Au—P1—C13B	105.5 (4)	C14—C15—H15A	110.1
C1—P1—C7	105.0 (5)	C14—C15—H15B	110.1
C1—P1—C13A	111.0 (7)	C14—C15—C16	107.8 (9)
C1—P1—C13B	93.8 (5)	H15A—C15—H15B	108.5
C7—P1—C13A	93.4 (5)	H15A—C15—C16	110.1
C7—P1—C13B	107.5 (6)	H15B—C15—C16	110.1
P1—C1—H1	105.7	C15—C16—H16A	109.0
P1—C1—C2	116.1 (8)	C15—C16—H16B	109.0
P1—C1—C6	113.6 (7)	C15—C16—C17	112.9 (12)
H1—C1—C2	105.7	H16A—C16—H16B	107.8
H1—C1—C6	105.7	H16A—C16—C17	109.0
C2—C1—C6	109.1 (8)	H16B—C16—C17	109.0
C1—C2—H2A	109.6	C16—C17—H17A	109.5
C1—C2—H2B	109.6	C16—C17—H17B	109.5
C1—C2—C3	110.1 (10)	C16—C17—C18	110.6 (12)
H2A—C2—H2B	108.2	H17A—C17—H17B	108.1
H2A—C2—C3	109.6	H17A—C17—C18	109.5
H2B—C2—C3	109.6	H17B—C17—C18	109.5
C2—C3—H3A	109.1	C17—C18—H18A	109.9
C2—C3—H3B	109.1	C17—C18—H18B	109.9
C2—C3—C4	112.6 (10)	C17—C18—C19	109.1 (9)
H3A—C3—H3B	107.8	H18A—C18—H18B	108.3
H3A—C3—C4	109.1	H18A—C18—C19	109.9
H3B—C3—C4	109.1	H18B—C18—C19	109.9
C3—C4—H4A	109.7	C14—C19—C18	115.0 (8)
C3—C4—H4B	109.7	C14—C19—H19A	108.5
C3—C4—C5	109.9 (10)	C14—C19—H19B	108.5
H4A—C4—H4B	108.2	C18—C19—H19A	108.5
H4A—C4—C5	109.7	C18—C19—H19B	108.5
H4B—C4—C5	109.7	H19A—C19—H19B	107.5
C4—C5—H5A	109.5	P2—C20—H20	106.0
C4—C5—H5B	109.5	P2—C20—C21	111.0 (7)

C4—C5—C6	110.8 (10)	P2—C20—C25	117.7 (8)
H5A—C5—H5B	108.1	H20—C20—C21	106.0
H5A—C5—C6	109.5	H20—C20—C25	106.0
H5B—C5—C6	109.5	C21—C20—C25	109.4 (9)
C1—C6—C5	113.9 (10)	C20—C21—H21A	109.7
C1—C6—H6A	108.8	C20—C21—H21B	109.7
C1—C6—H6B	108.8	C20—C21—C22	109.8 (9)
C5—C6—H6A	108.8	H21A—C21—H21B	108.2
C5—C6—H6B	108.8	H21A—C21—C22	109.7
H6A—C6—H6B	107.7	H21B—C21—C22	109.7
P1—C7—H7	107.5	C21—C22—H22A	109.5
P1—C7—C8	112.4 (8)	C21—C22—H22B	109.5
P1—C7—C12	111.9 (7)	C21—C22—C23	110.6 (12)
H7—C7—C8	107.5	H22A—C22—H22B	108.1
H7—C7—C12	107.5	H22A—C22—C23	109.5
C8—C7—C12	109.8 (11)	H22B—C22—C23	109.5
C7—C8—H8A	109.4	C22—C23—H23A	109.2
C7—C8—H8B	109.4	C22—C23—H23B	109.2
C7—C8—C9	111.3 (11)	C22—C23—C24	112.2 (10)
H8A—C8—H8B	108.0	H23A—C23—H23B	107.9
H8A—C8—C9	109.4	H23A—C23—C24	109.2
H8B—C8—C9	109.4	H23B—C23—C24	109.2
C8—C9—H9A	109.4	C23—C24—H24A	109.7
C8—C9—H9B	109.4	C23—C24—H24B	109.7
C8—C9—C10	111.3 (11)	C23—C24—C25	109.9 (11)
H9A—C9—H9B	108.0	H24A—C24—H24B	108.2
H9A—C9—C10	109.4	H24A—C24—C25	109.7
H9B—C9—C10	109.4	H24B—C24—C25	109.7
C9—C10—H10A	109.6	C20—C25—C24	112.3 (11)
C9—C10—H10B	109.6	C20—C25—H25A	109.2
C9—C10—C11	110.1 (12)	C20—C25—H25B	109.2
H10A—C10—H10B	108.2	C24—C25—H25A	109.2
H10A—C10—C11	109.6	C24—C25—H25B	109.2
H10B—C10—C11	109.6	H25A—C25—H25B	107.9
C10—C11—H11A	109.0	P2—C26A—C26A^{i}	113.8 (10)
C10—C11—H11B	109.0	P2—C26A—H26A	108.8
C10—C11—C12	113.0 (10)	P2—C26A—H26B	108.8
H11A—C11—H11B	107.8	C26A^{i}—C26A—H26A	108.8
H11A—C11—C12	109.0	C26A^{i}—C26A—H26B	108.8
H11B—C11—C12	109.0	H26A—C26A—H26B	107.7
C7—C12—C11	108.1 (8)	P2—C26B—C26B^{i}	114.0 (11)
C7—C12—H12A	110.1	P2—C26B—H26C	108.8
C7—C12—H12B	110.1	P2—C26B—H26D	108.8
C11—C12—H12A	110.1	C26B^{i}—C26B—H26C	108.8
C11—C12—H12B	110.1	C26B^{i}—C26B—H26D	108.8
H12A—C12—H12B	108.4	H26C—C26B—H26D	107.6
P1—C13A—C13A^{i}	112.4 (9)	H27—C27—Cl2	108.1
P1—C13A—H13A	109.1	H27—C27—Cl3	108.1

P1—C13A—H13B	109.1	H27—C27—Cl4	108.1
C13A^{i}—C13A—H13A	109.1	Cl2—C27—Cl3	111.2 (7)
C13A^{i}—C13A—H13B	109.1	Cl2—C27—Cl4	109.3 (7)
H13A—C13A—H13B	107.9	Cl3—C27—Cl4	111.8 (7)
P1—C13B—C13B^{i}	113.3 (7)	H28—C28—Cl5	105.5
P1—C13B—H13C	108.9	H28—C28—Cl6	105.5
P1—C13B—H13D	108.9	H28—C28—Cl7	105.5
C13B^{i}—C13B—H13C	108.9	H28—C28—Cl5X	121.9
C13B^{i}—C13B—H13D	108.9	H28—C28—Cl6X	94.7
H13C—C13B—H13D	107.7	H28—C28—Cl7X	107.9
Au—P2—C14	126.5 (3)	Cl5—C28—Cl6	113.1 (8)
Au—P2—C20	115.1 (3)	Cl5—C28—Cl7	104.0 (6)
Au—P2—C26A	102.6 (5)	Cl6—C28—Cl7	122.0 (9)
Au—P2—C26B	102.7 (5)	Cl5X—C28—Cl6X	112.5 (7)
C14—P2—C20	101.3 (4)	Cl5X—C28—Cl7X	102.4 (6)
C14—P2—C26A	111.6 (8)	Cl6X—C28—Cl7X	118.5 (8)

P1^{i}—Au—P1—C1	111.1 (4)	P1—Au—P2—C14	0.5 (4)
P1^{i}—Au—P1—C7	−116.4 (4)	P1^{i}—Au—P2—C14	106.6 (4)
P1^{i}—Au—P1—C13A	−10.6 (6)	P1—Au—P2—C20	−127.5 (4)
P1^{i}—Au—P1—C13B	9.7 (5)	P1^{i}—Au—P2—C20	−21.4 (4)
P2—Au—P1—C1	−130.9 (3)	P1—Au—P2—C26A	130.0 (7)
P2^{i}—Au—P1—C1	−22.4 (4)	P1^{i}—Au—P2—C26A	−123.9 (7)
P2—Au—P1—C7	1.6 (4)	P1—Au—P2—C26B	109.1 (8)
P2^{i}—Au—P1—C7	110.1 (4)	P1^{i}—Au—P2—C26B	−144.7 (8)
P2—Au—P1—C13A	107.4 (6)	P2^{i}—Au—P2—C14	−119.0 (4)
P2^{i}—Au—P1—C13A	−144.1 (6)	P2^{i}—Au—P2—C20	113.0 (4)
P2—Au—P1—C13B	127.7 (5)	P2^{i}—Au—P2—C26A	10.5 (7)
P2^{i}—Au—P1—C13B	−123.8 (5)	P2^{i}—Au—P2—C26B	−10.3 (7)
Au—P1—C1—C2	−171.8 (7)	Au—P2—C14—C15	47.7 (11)
Au—P1—C1—C6	−44.0 (8)	Au—P2—C14—C19	−76.9 (8)
C7—P1—C1—C2	46.3 (9)	C20—P2—C14—C15	−179.0 (10)
C7—P1—C1—C6	174.1 (7)	C20—P2—C14—C19	56.4 (9)
C13A—P1—C1—C2	−53.4 (9)	C26A—P2—C14—C15	−78.2 (11)
C13A—P1—C1—C6	74.4 (8)	C26A—P2—C14—C19	157.3 (8)
C13B—P1—C1—C2	−63.0 (9)	C26B—P2—C14—C15	−63.7 (12)
C13B—P1—C1—C6	64.8 (8)	C26B—P2—C14—C19	171.7 (11)
P1—C1—C2—C3	−174.3 (8)	P2—C14—C15—C16	177.0 (12)
C6—C1—C2—C3	55.7 (13)	C19—C14—C15—C16	−55.3 (16)
C1—C2—C3—C4	−58.2 (14)	C14—C15—C16—C17	57.3 (19)
C2—C3—C4—C5	56.5 (16)	C15—C16—C17—C18	−58.0 (17)
C3—C4—C5—C6	−53.7 (15)	C16—C17—C18—C19	54.2 (15)
C4—C5—C6—C1	55.4 (13)	P2—C14—C19—C18	−177.0 (7)
P1—C1—C6—C5	172.5 (8)	C15—C14—C19—C18	57.9 (12)
C2—C1—C6—C5	−56.1 (12)	C17—C18—C19—C14	−56.8 (14)
Au—P1—C7—C8	45.4 (11)	Au—P2—C20—C21	−45.4 (9)
Au—P1—C7—C12	−78.7 (9)	Au—P2—C20—C25	−172.5 (7)
C1—P1—C7—C8	−178.8 (10)	C14—P2—C20—C21	174.8 (8)

C1—P1—C7—C12	57.1 (9)	C14—P2—C20—C25	47.7 (9)
C13A—P1—C7—C8	−66.0 (12)	C26A—P2—C20—C21	61.4 (10)
C13A—P1—C7—C12	169.9 (10)	C26A—P2—C20—C25	−65.7 (10)
C13B—P1—C7—C8	−79.8 (11)	C26B—P2—C20—C21	72.3 (9)
C13B—P1—C7—C12	156.1 (8)	C26B—P2—C20—C25	−54.9 (9)
P1—C7—C8—C9	176.9 (12)	P2—C20—C21—C22	171.2 (9)
C12—C7—C8—C9	−57.8 (16)	C25—C20—C21—C22	−57.3 (13)
C7—C8—C9—C10	55.7 (19)	C20—C21—C22—C23	58.1 (13)
C8—C9—C10—C11	−54.2 (17)	C21—C22—C23—C24	−57.9 (17)
C9—C10—C11—C12	57.5 (13)	C22—C23—C24—C25	55.6 (18)
P1—C7—C12—C11	−176.3 (8)	C23—C24—C25—C20	−55.5 (15)
C8—C7—C12—C11	58.2 (12)	P2—C20—C25—C24	−175.3 (9)
C10—C11—C12—C7	−59.3 (13)	C21—C20—C25—C24	56.8 (13)
Au—P1—C13A—C13A^{i}	38 (2)	Au—P2—C26A—C26A^{i}	−38 (2)
C1—P1—C13A—C13A^{i}	−86.0 (19)	C14—P2—C26A—C26A^{i}	100 (2)
C7—P1—C13A—C13A^{i}	166.5 (19)	C20—P2—C26A—C26A^{i}	−155 (2)
Au—P1—C13B—C13B^{i}	−35.3 (17)	Au—P2—C26B—C26B^{i}	37 (2)
C1—P1—C13B—C13B^{i}	−151.4 (16)	C14—P2—C26B—C26B^{i}	167 (2)
C7—P1—C13B—C13B^{i}	101.5 (16)	C20—P2—C26B—C26B^{i}	−87 (2)

Symmetry code: (i) $-x$, y, $-z+1/2$.