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[2-(Diphenylphosphino-κP)benzaldehyde]gold(I) chloride

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.009 Å
R factor = 0.037
wR factor = 0.100
Data-to-parameter ratio = 18.6

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

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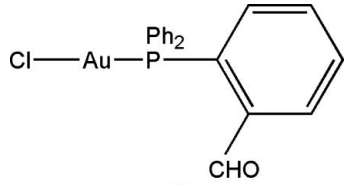
The title compound, [AuCl{(2-$(C_6H_5)_2PC_6H_4CHO$}], crystallizes with two molecules in the asymmetric unit. A comparison of the Au—P, Au—Cl and Cl—Au—P bond lengths and angles for both independent molecules with those of the previously reported compounds ClAu(2-$Ph_2PC_6H_4X$) (X = H, $OSiMe_3$ or OH) reveals that the nature of the *ortho* X substituent has a negligible effect on these structural parameters.

Comment

Functionalized tertiary phosphines bearing an additional hard oxygen donor group continue to find a range of uses in coordination and organometallic chemistry and catalysis (Downing & Smith, 2004). One classic example of such a hybrid ligand is 2-(diphenylphosphino)benzaldehyde (Hoots *et al.*, 1982; Chandrasekaran *et al.*, 2001), which has been studied in conjunction with a range of transition metal centres, *e.g.* W, Re, Rh and Cu (Yeh *et al.*, 2004, 2006; Chen *et al.*, 2001; Mail *et al.*, 2000). Furthermore, 2-$Ph_2PC_6H_4CHO$ undergoes Schiff base condensation reactions with primary amines to give a range of polydentate ligands containing, amongst others, PNO or PNSe donor sets (Bhattacharyya *et al.*, 1998; Durran *et al.*, 2002). We present here the structure of the title linear gold(I) complex, (I). Recently, trigonal and tetrahedral copper(I) complexes with 2-$Ph_2PC_6H_4CHO$ have been reported (Yeh *et al.*, 2006).



(I)

Compound (I), ClAu[2-$(C_6H_5)_2PC_6H_4CHO$], crystallizes in a centrosymmetric space group, the asymmetric unit containing two independent molecules (Figs. 1 and 2, Table 1). The crystal structure of (I) confirms an essentially linear arrangement of both chloride and tertiary phosphine ligands around the gold(I) metal centre. In (I), the Au—P and Au—Cl bond lengths for both independent moleules are typical for this class of compound and agree well with those reported for related complexes (Table 2) (Hollatz *et al.*, 1999; Baenziger *et al.*, 1976).

Recently, it has been shown by X-ray diffraction that, in uncoordinated 2-$Ph_2PC_6H_4CHO$, the carbonyl group resides in close proximity to the P atom and the C=O distance is 1.194 (3) Å [*cf.* 1.207 (7) and 1.219 (7) Å in (I)]. The Au···O separations in (I) are 3.109 (4) and 3.106 (4) Å, shorter than

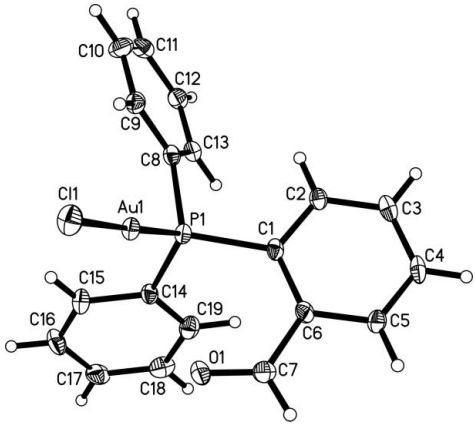


Figure 1
A perspective view of the complex containing Au1, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

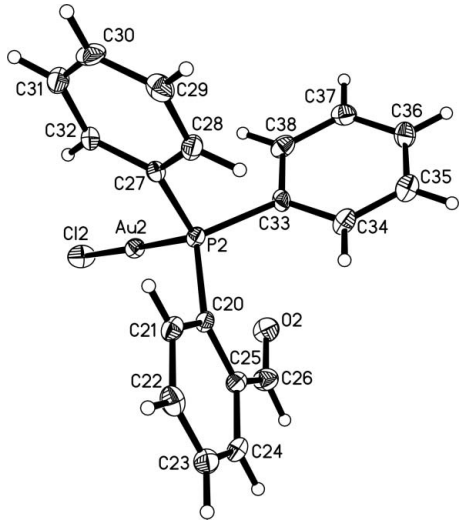


Figure 2
A perspective view of the complex containing Au2, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

the sum of their van der Waals radii of *ca* 3.2 Å, suggesting weak additional coordination. The shortest Au···Au intermolecular separation is 5.5900 (4) Å, indicating extremely weak aurophilicity. The dihedral angle between the formyl group and the benzene ring is 3.0 (7)° in the complex containing Au1, and 2.4 (5)° in the complex containing Au2.

Weak intermolecular hydrogen bonds are observed between phenyl CH groups and the coordinated Cl ligands, with C···Cl distances in the range 3.6–3.8 Å.

In summary, we have shown that the known ligand 2-$Ph_2PC_6H_4CHO$ can be complexed to gold(I), affording a classic two-coordinate complex with typical Au—P and Au—Cl bond lengths and Cl—Au—P bond angles.

Experimental

The preparation of (I) was carried out as follows. To a CH_2Cl_2 (10 ml) solution of AuCl(tht) (tht is tetrahydrothiophene; 0.048 g, 0.150 mmol) was added 2-$Ph_2PC_6H_4CHO$ (0.047 g, 0.162 mmol). The yellow solution was stirred for 10 min and the volume reduced to *ca* 2–3 ml under reduced pressure. Addition of diethyl ether (10 ml) and petroleum ether (b.p. 333–353 K, 20 ml) gave (I), which was collected by suction filtration and dried *in vacuo* (yield 0.068 g, 87%). Selected spectroscopic data: $^{31}P\{^1H\}$ NMR ($CDCl_3$, δ, p.p.m.): 32.2; ^1H NMR ($CDCl_3$, δ, p.p.m.): 10.26 (CHO), 8.10–6.94 (arom. H); FT–IR (ν, cm^{-1}): 1698 (CO), 1678 (CO), 333 (AuCl). Analysis, found: C 43.89, H 2.62%; $C_{19}H_{15}AuClOP$ requires: C 43.65, H 2.90%. Colourless block crystals of (I) were obtained by vapour diffusion of diethyl ether into a $CDCl_3$ solution.

Crystal data

$[AuCl(C_{19}H_{15}OP)]$	V = 1677.96 (6) Å^3
M_r = 522.70	Z = 4
Triclinic, $P\overline{1}$	D_x = 2.069 Mg m^{-3}
a = 10.2431 (2) Å	Mo $K\alpha$ radiation
b = 10.4949 (2) Å	μ = 9.02 mm^{-1}
c = 16.6533 (3) Å	T = 120 (2) K
α = 97.1857 (7)°	Plate, colourless
β = 103.5519 (9)°	0.25 × 0.20 × 0.04 mm
γ = 101.4375 (9)°	

Data collection

Bruker Nonius KappaCCD area-detector diffractometer	(*SORTAV*; Blessing, 1995)
	T_{min} = 0.128, T_{max} = 0.697
φ and ω scans	29712 measured reflections
Absorption correction: multi-scan using multiple and symmetry-related data measurements	7704 independent reflections
	6936 reflections with $I > 2\sigma(I)$
	R_{int} = 0.063
	θ_{max} = 27.7°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 5.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	
$wR(F^2)$ = 0.100	
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.002
7704 reflections	$\Delta\rho_{max}$ = 3.10 e Å^{-3}
415 parameters	$\Delta\rho_{min}$ = −1.40 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Au1—P1	2.2297 (13)	Au2—P2	2.2304 (14)
Au1—Cl1	2.2819 (13)	Au2—Cl2	2.2836 (14)
P1—C14	1.822 (5)	P2—C33	1.807 (5)
P1—C1	1.825 (5)	P2—C27	1.817 (6)
P1—C8	1.827 (5)	P2—C20	1.838 (5)
C7—O1	1.207 (7)	C26—O2	1.219 (7)
P1—Au1—Cl1	178.79 (5)	P2—Au2—Cl2	178.12 (5)

Table 2
Selected bond lengths and angles (Å, °) taken from compounds of the form ClAu(2-$Ph_2PC_6H_4X$) [X = H (Baenziger *et al.*, 1976), $OSiMe_3$ or OH (Hollatz *et al.*, 1999)].

	X = H	X = OH	X = $OSiMe_3$
Au—P	2.235 (3)	2.2226 (2)	2.2294 (8)
Au—Cl	2.279 (3)	2.285 (2)	2.2851 (8)
P—Au—Cl	179.68 (8)	176.85 (8)	177.30 (3)

H atoms were placed in geometric positions using a riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The maximum and minimum electron-density peaks are located 0.88 Å from Au1 and 0.70 Å from Au2, respectively.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); 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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Crystal data

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M_r = 522.70
Triclinic, $P\overline{1}$
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α = 97.1857 (7)°
β = 103.5519 (9)°
γ = 101.4375 (9)°
V = 1677.96 (6) Å^3
Z = 4
F(000) = 992
D_x = 2.069 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 61735 reflections
θ = 2.9–27.5°
μ = 9.02 mm^{-1}
T = 120 K
Thick plate, colourless
0.25 × 0.20 × 0.04 mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer
Radiation source: Enraf Nonius FR591 rotating anode
10cm confocal mirrors monochromator
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φ and ω scans
Absorption correction: multi-scan using multiple and symmetry-related data measurements (SORTAV; Blessing, 1995)
T_{min} = 0.128, T_{max} = 0.697
29712 measured reflections
7704 independent reflections
6936 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 27.7°, θ_{min} = 2.9°
h = −13→13
k = −13→13
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.06
7704 reflections
415 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
$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 5.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 3.10 e Å^{-3}
$\Delta\rho_{min}$ = −1.40 e Å^{-3}

Special details

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

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Au1	0.69934 (2)	0.116173 (19)	0.424881 (11)	0.01437 (7)
Cl1	0.65437 (14)	0.03133 (14)	0.28557 (8)	0.0213 (3)
P1	0.73885 (14)	0.19673 (13)	0.56099 (8)	0.0134 (3)
C1	0.8005 (5)	0.0849 (5)	0.6285 (3)	0.0148 (10)
C2	0.7170 (6)	0.0265 (5)	0.6749 (3)	0.0159 (10)
H2	0.6295	0.0461	0.6716	0.019*
C3	0.7597 (6)	−0.0604 (5)	0.7263 (3)	0.0201 (11)
H3	0.7004	−0.1005	0.7569	0.024*
C4	0.8878 (6)	−0.0890 (6)	0.7333 (4)	0.0225 (12)
H4	0.9180	−0.1464	0.7696	0.027*
C5	0.9703 (6)	−0.0332 (5)	0.6869 (4)	0.0191 (11)
H5	1.0577	−0.0533	0.6908	0.023*
C6	0.9285 (6)	0.0528 (5)	0.6339 (3)	0.0170 (10)
C7	1.0229 (6)	0.1008 (5)	0.5849 (3)	0.0183 (11)
H7	1.1072	0.0731	0.5933	0.022*
O1	1.0025 (4)	0.1729 (4)	0.5346 (2)	0.0205 (8)
C8	0.5803 (6)	0.2252 (5)	0.5844 (3)	0.0163 (10)
C9	0.4615 (6)	0.1980 (5)	0.5197 (3)	0.0184 (11)
H9	0.4607	0.1564	0.4655	0.022*
C10	0.3421 (6)	0.2316 (6)	0.5336 (4)	0.0245 (12)
H10	0.2603	0.2129	0.4888	0.029*
C11	0.3431 (6)	0.2918 (6)	0.6123 (4)	0.0217 (12)
H11	0.2625	0.3157	0.6217	0.026*
C12	0.4626 (6)	0.3173 (6)	0.6780 (4)	0.0202 (11)
H12	0.4630	0.3574	0.7325	0.024*
C13	0.5815 (6)	0.2844 (5)	0.6641 (3)	0.0182 (11)
H13	0.6632	0.3023	0.7089	0.022*
C14	0.8589 (5)	0.3577 (5)	0.6010 (3)	0.0156 (10)
C15	0.8508 (6)	0.4559 (6)	0.5518 (4)	0.0212 (11)
H15	0.7859	0.4366	0.4982	0.025*
C16	0.9366 (7)	0.5807 (6)	0.5808 (4)	0.0271 (13)
H16	0.9299	0.6473	0.5473	0.032*
C17	1.0325 (6)	0.6093 (6)	0.6586 (4)	0.0248 (12)
H17	1.0924	0.6948	0.6782	0.030*
C18	1.0402 (6)	0.5130 (6)	0.7074 (4)	0.0232 (12)

H18	1.1059	0.5326	0.7608	0.028*
C19	0.9529 (6)	0.3871 (6)	0.6796 (4)	0.0205 (11)
H19	0.9577	0.3218	0.7143	0.025*
Au2	1.02900 (2)	0.690763 (19)	0.904323 (12)	0.01608 (7)
Cl2	1.24726 (15)	0.77100 (15)	0.89367 (9)	0.0260 (3)
P2	0.81313 (14)	0.61296 (13)	0.91035 (8)	0.0144 (3)
C20	0.7804 (5)	0.6774 (5)	1.0097 (3)	0.0146 (10)
C21	0.7514 (6)	0.5895 (5)	1.0624 (4)	0.0182 (11)
H21	0.7419	0.4978	1.0447	0.022*
C22	0.7360 (6)	0.6354 (6)	1.1419 (4)	0.0222 (12)
H22	0.7164	0.5743	1.1775	0.027*
C23	0.7489 (6)	0.7667 (6)	1.1685 (4)	0.0218 (11)
H23	0.7374	0.7969	1.2220	0.026*
C24	0.7788 (6)	0.8559 (6)	1.1167 (4)	0.0210 (11)
H24	0.7892	0.9475	1.1355	0.025*
C25	0.7937 (6)	0.8128 (5)	1.0380 (3)	0.0179 (11)
C26	0.8287 (6)	0.9151 (6)	0.9893 (4)	0.0229 (12)
H26	0.8349	1.0040	1.0130	0.027*
O2	0.8505 (4)	0.8949 (4)	0.9205 (3)	0.0248 (9)
C27	0.7707 (6)	0.4343 (5)	0.9010 (3)	0.0161 (10)
C28	0.6382 (6)	0.3653 (6)	0.8953 (3)	0.0193 (11)
H28	0.5688	0.4120	0.8991	0.023*
C29	0.6054 (7)	0.2272 (6)	0.8841 (4)	0.0238 (12)
H29	0.5147	0.1802	0.8816	0.029*
C30	0.7064 (6)	0.1600 (5)	0.8768 (4)	0.0228 (12)
H30	0.6845	0.0662	0.8692	0.027*
C31	0.8379 (6)	0.2264 (6)	0.8803 (4)	0.0239 (12)
H31	0.9055	0.1788	0.8735	0.029*
C32	0.8715 (6)	0.3641 (6)	0.8938 (3)	0.0188 (11)
H32	0.9632	0.4105	0.8983	0.023*
C33	0.6813 (5)	0.6367 (5)	0.8240 (3)	0.0160 (10)
C34	0.5582 (6)	0.6684 (6)	0.8326 (4)	0.0210 (11)
H34	0.5423	0.6830	0.8866	0.025*
C35	0.4597 (6)	0.6786 (6)	0.7625 (4)	0.0246 (12)
H35	0.3773	0.7024	0.7685	0.030*
C36	0.4815 (6)	0.6542 (6)	0.6840 (4)	0.0230 (12)
H36	0.4138	0.6613	0.6360	0.028*
C37	0.6008 (6)	0.6195 (6)	0.6745 (3)	0.0214 (11)
H37	0.6135	0.6009	0.6200	0.026*
C38	0.7025 (6)	0.6114 (5)	0.7442 (4)	0.0207 (11)
H38	0.7853	0.5891	0.7377	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Au1	0.01748 (12)	0.01383 (11)	0.01319 (11)	0.00591 (8)	0.00416 (8)	0.00383 (8)
Cl1	0.0279 (7)	0.0228 (7)	0.0147 (6)	0.0096 (6)	0.0064 (5)	0.0021 (5)
P1	0.0155 (6)	0.0126 (6)	0.0125 (6)	0.0045 (5)	0.0031 (5)	0.0032 (5)

C1	0.018 (3)	0.007 (2)	0.016 (2)	0.0006 (19)	0.000 (2)	0.0015 (18)
C2	0.020 (3)	0.011 (2)	0.018 (2)	0.004 (2)	0.005 (2)	0.0029 (19)
C3	0.030 (3)	0.015 (3)	0.017 (3)	0.003 (2)	0.008 (2)	0.006 (2)
C4	0.031 (3)	0.017 (3)	0.022 (3)	0.006 (2)	0.006 (2)	0.011 (2)
C5	0.020 (3)	0.013 (2)	0.026 (3)	0.007 (2)	0.006 (2)	0.006 (2)
C6	0.017 (3)	0.009 (2)	0.021 (3)	−0.001 (2)	0.001 (2)	0.003 (2)
C7	0.017 (3)	0.015 (3)	0.022 (3)	0.004 (2)	0.006 (2)	0.002 (2)
O1	0.023 (2)	0.0184 (19)	0.024 (2)	0.0053 (16)	0.0086 (16)	0.0097 (16)
C8	0.018 (3)	0.012 (2)	0.020 (3)	0.004 (2)	0.005 (2)	0.006 (2)
C9	0.020 (3)	0.016 (3)	0.020 (3)	0.005 (2)	0.004 (2)	0.005 (2)
C10	0.015 (3)	0.025 (3)	0.030 (3)	0.004 (2)	0.001 (2)	0.005 (2)
C11	0.019 (3)	0.018 (3)	0.035 (3)	0.008 (2)	0.015 (2)	0.008 (2)
C12	0.022 (3)	0.018 (3)	0.022 (3)	0.005 (2)	0.008 (2)	0.005 (2)
C13	0.019 (3)	0.018 (3)	0.018 (3)	0.004 (2)	0.005 (2)	0.007 (2)
C14	0.018 (3)	0.012 (2)	0.019 (3)	0.005 (2)	0.006 (2)	0.005 (2)
C15	0.027 (3)	0.019 (3)	0.020 (3)	0.008 (2)	0.005 (2)	0.008 (2)
C16	0.033 (3)	0.019 (3)	0.032 (3)	0.004 (3)	0.012 (3)	0.014 (2)
C17	0.020 (3)	0.014 (3)	0.039 (3)	0.001 (2)	0.009 (3)	0.004 (2)
C18	0.020 (3)	0.018 (3)	0.029 (3)	0.005 (2)	0.005 (2)	−0.003 (2)
C19	0.024 (3)	0.018 (3)	0.022 (3)	0.010 (2)	0.007 (2)	0.004 (2)
Au2	0.01753 (12)	0.01563 (12)	0.01621 (11)	0.00452 (8)	0.00588 (8)	0.00346 (8)
Cl2	0.0233 (7)	0.0265 (7)	0.0280 (7)	0.0003 (6)	0.0128 (6)	0.0014 (6)
P2	0.0158 (6)	0.0140 (6)	0.0153 (6)	0.0055 (5)	0.0054 (5)	0.0039 (5)
C20	0.015 (2)	0.015 (2)	0.016 (2)	0.006 (2)	0.0046 (19)	0.0037 (19)
C21	0.015 (3)	0.016 (3)	0.024 (3)	0.004 (2)	0.006 (2)	0.003 (2)
C22	0.017 (3)	0.028 (3)	0.022 (3)	0.005 (2)	0.006 (2)	0.009 (2)
C23	0.023 (3)	0.025 (3)	0.020 (3)	0.008 (2)	0.007 (2)	0.004 (2)
C24	0.022 (3)	0.020 (3)	0.024 (3)	0.011 (2)	0.006 (2)	0.003 (2)
C25	0.021 (3)	0.018 (3)	0.016 (3)	0.008 (2)	0.005 (2)	0.003 (2)
C26	0.029 (3)	0.020 (3)	0.021 (3)	0.007 (2)	0.008 (2)	0.004 (2)
O2	0.033 (2)	0.023 (2)	0.023 (2)	0.0084 (18)	0.0109 (18)	0.0084 (17)
C27	0.019 (3)	0.016 (3)	0.013 (2)	0.007 (2)	0.001 (2)	0.0032 (19)
C28	0.021 (3)	0.021 (3)	0.019 (3)	0.010 (2)	0.006 (2)	0.006 (2)
C29	0.027 (3)	0.021 (3)	0.020 (3)	0.002 (2)	0.001 (2)	0.008 (2)
C30	0.034 (3)	0.011 (2)	0.022 (3)	0.003 (2)	0.006 (2)	0.002 (2)
C31	0.026 (3)	0.027 (3)	0.021 (3)	0.015 (2)	0.004 (2)	0.004 (2)
C32	0.017 (3)	0.021 (3)	0.019 (3)	0.009 (2)	0.001 (2)	0.003 (2)
C33	0.018 (3)	0.014 (2)	0.016 (2)	0.005 (2)	0.001 (2)	0.007 (2)
C34	0.025 (3)	0.022 (3)	0.022 (3)	0.012 (2)	0.012 (2)	0.009 (2)
C35	0.025 (3)	0.024 (3)	0.029 (3)	0.010 (2)	0.009 (2)	0.007 (2)
C36	0.027 (3)	0.021 (3)	0.022 (3)	0.010 (2)	0.002 (2)	0.009 (2)
C37	0.030 (3)	0.018 (3)	0.016 (3)	0.005 (2)	0.006 (2)	0.004 (2)
C38	0.027 (3)	0.017 (3)	0.022 (3)	0.008 (2)	0.011 (2)	0.006 (2)

Geometric parameters (Å, º)

Au1—P1	2.2297 (13)	Au2—P2	2.2304 (14)
Au1—Cl1	2.2819 (13)	Au2—Cl2	2.2836 (14)

P1—C14	1.822 (5)	P2—C33	1.807 (5)
P1—C1	1.825 (5)	P2—C27	1.817 (6)
P1—C8	1.827 (5)	P2—C20	1.838 (5)
C1—C2	1.388 (7)	C20—C21	1.388 (7)
C1—C6	1.402 (8)	C20—C25	1.409 (7)
C2—C3	1.389 (7)	C21—C22	1.406 (8)
C2—H2	0.9500	C21—H21	0.9500
C3—C4	1.386 (8)	C22—C23	1.364 (8)
C3—H3	0.9500	C22—H22	0.9500
C4—C5	1.370 (8)	C23—C24	1.387 (8)
C4—H4	0.9500	C23—H23	0.9500
C5—C6	1.396 (7)	C24—C25	1.385 (8)
C5—H5	0.9500	C24—H24	0.9500
C6—C7	1.461 (8)	C25—C26	1.465 (8)
C7—O1	1.207 (7)	C26—O2	1.219 (7)
C7—H7	0.9500	C26—H26	0.9500
C8—C9	1.376 (8)	C27—C28	1.381 (8)
C8—C13	1.389 (7)	C27—C32	1.400 (7)
C9—C10	1.399 (8)	C28—C29	1.399 (8)
C9—H9	0.9500	C28—H28	0.9500
C10—C11	1.379 (8)	C29—C30	1.382 (9)
C10—H10	0.9500	C29—H29	0.9500
C11—C12	1.391 (8)	C30—C31	1.372 (9)
C11—H11	0.9500	C30—H30	0.9500
C12—C13	1.391 (8)	C31—C32	1.394 (8)
C12—H12	0.9500	C31—H31	0.9500
C13—H13	0.9500	C32—H32	0.9500
C14—C19	1.388 (8)	C33—C38	1.398 (7)
C14—C15	1.398 (7)	C33—C34	1.400 (8)
C15—C16	1.382 (8)	C34—C35	1.383 (8)
C15—H15	0.9500	C34—H34	0.9500
C16—C17	1.387 (9)	C35—C36	1.379 (8)
C16—H16	0.9500	C35—H35	0.9500
C17—C18	1.377 (9)	C36—C37	1.379 (8)
C17—H17	0.9500	C36—H36	0.9500
C18—C19	1.395 (8)	C37—C38	1.390 (8)
C18—H18	0.9500	C37—H37	0.9500
C19—H19	0.9500	C38—H38	0.9500

P1—Au1—Cl1	178.79 (5)	P2—Au2—Cl2	178.12 (5)
C14—P1—C1	106.5 (2)	C33—P2—C27	101.7 (2)
C14—P1—C8	102.6 (2)	C33—P2—C20	109.0 (2)
C1—P1—C8	106.9 (2)	C27—P2—C20	105.5 (2)
C14—P1—Au1	116.77 (18)	C33—P2—Au2	114.41 (18)
C1—P1—Au1	112.69 (17)	C27—P2—Au2	112.05 (18)
C8—P1—Au1	110.53 (18)	C20—P2—Au2	113.34 (18)
C2—C1—C6	118.3 (5)	C21—C20—C25	118.2 (5)
C2—C1—P1	119.2 (4)	C21—C20—P2	118.3 (4)

C6—C1—P1	122.5 (4)	C25—C20—P2	123.3 (4)
C1—C2—C3	120.9 (5)	C20—C21—C22	120.4 (5)
C1—C2—H2	119.5	C20—C21—H21	119.8
C3—C2—H2	119.5	C22—C21—H21	119.8
C4—C3—C2	120.6 (5)	C23—C22—C21	120.7 (5)
C4—C3—H3	119.7	C23—C22—H22	119.6
C2—C3—H3	119.7	C21—C22—H22	119.6
C5—C4—C3	118.9 (5)	C22—C23—C24	119.5 (5)
C5—C4—H4	120.5	C22—C23—H23	120.2
C3—C4—H4	120.5	C24—C23—H23	120.2
C4—C5—C6	121.4 (5)	C25—C24—C23	120.7 (5)
C4—C5—H5	119.3	C25—C24—H24	119.6
C6—C5—H5	119.3	C23—C24—H24	119.6
C5—C6—C1	119.9 (5)	C24—C25—C20	120.4 (5)
C5—C6—C7	116.0 (5)	C24—C25—C26	116.4 (5)
C1—C6—C7	124.0 (5)	C20—C25—C26	123.2 (5)
O1—C7—C6	125.3 (5)	O2—C26—C25	124.9 (5)
O1—C7—H7	117.4	O2—C26—H26	117.6
C6—C7—H7	117.4	C25—C26—H26	117.6
C9—C8—C13	120.1 (5)	C28—C27—C32	119.1 (5)
C9—C8—P1	118.6 (4)	C28—C27—P2	121.2 (4)
C13—C8—P1	121.0 (4)	C32—C27—P2	119.6 (4)
C8—C9—C10	120.2 (5)	C27—C28—C29	120.7 (5)
C8—C9—H9	119.9	C27—C28—H28	119.7
C10—C9—H9	119.9	C29—C28—H28	119.7
C11—C10—C9	120.0 (5)	C30—C29—C28	119.2 (6)
C11—C10—H10	120.0	C30—C29—H29	120.4
C9—C10—H10	120.0	C28—C29—H29	120.4
C10—C11—C12	119.8 (5)	C31—C30—C29	121.1 (5)
C10—C11—H11	120.1	C31—C30—H30	119.4
C12—C11—H11	120.1	C29—C30—H30	119.4
C11—C12—C13	120.2 (5)	C30—C31—C32	119.6 (5)
C11—C12—H12	119.9	C30—C31—H31	120.2
C13—C12—H12	119.9	C32—C31—H31	120.2
C8—C13—C12	119.8 (5)	C31—C32—C27	120.3 (5)
C8—C13—H13	120.1	C31—C32—H32	119.8
C12—C13—H13	120.1	C27—C32—H32	119.8
C19—C14—C15	119.4 (5)	C38—C33—C34	119.8 (5)
C19—C14—P1	122.3 (4)	C38—C33—P2	116.2 (4)
C15—C14—P1	118.2 (4)	C34—C33—P2	123.8 (4)
C16—C15—C14	120.3 (6)	C35—C34—C33	120.1 (5)
C16—C15—H15	119.9	C35—C34—H34	120.0
C14—C15—H15	119.9	C33—C34—H34	120.0
C15—C16—C17	120.2 (5)	C36—C35—C34	119.9 (5)
C15—C16—H16	119.9	C36—C35—H35	120.1
C17—C16—H16	119.9	C34—C35—H35	120.1
C18—C17—C16	119.6 (5)	C37—C36—C35	120.6 (5)
C18—C17—H17	120.2	C37—C36—H36	119.7

C16—C17—H17	120.2	C35—C36—H36	119.7
C17—C18—C19	120.9 (6)	C36—C37—C38	120.6 (5)
C17—C18—H18	119.6	C36—C37—H37	119.7
C19—C18—H18	119.6	C38—C37—H37	119.7
C14—C19—C18	119.6 (5)	C37—C38—C33	119.1 (5)
C14—C19—H19	120.2	C37—C38—H38	120.4
C18—C19—H19	120.2	C33—C38—H38	120.4

C14—P1—C1—C2	117.8 (4)	C33—P2—C20—C21	117.1 (4)
C8—P1—C1—C2	8.6 (5)	C27—P2—C20—C21	8.7 (5)
Au1—P1—C1—C2	−113.0 (4)	Au2—P2—C20—C21	−114.2 (4)
C14—P1—C1—C6	−63.7 (5)	C33—P2—C20—C25	−68.0 (5)
C8—P1—C1—C6	−172.9 (4)	C27—P2—C20—C25	−176.4 (4)
Au1—P1—C1—C6	65.5 (5)	Au2—P2—C20—C25	60.6 (5)
C6—C1—C2—C3	0.7 (8)	C25—C20—C21—C22	0.0 (8)
P1—C1—C2—C3	179.3 (4)	P2—C20—C21—C22	175.1 (4)
C1—C2—C3—C4	1.0 (8)	C20—C21—C22—C23	0.2 (8)
C2—C3—C4—C5	−1.8 (9)	C21—C22—C23—C24	−0.6 (9)
C3—C4—C5—C6	0.9 (9)	C22—C23—C24—C25	0.9 (9)
C4—C5—C6—C1	0.9 (8)	C23—C24—C25—C20	−0.8 (8)
C4—C5—C6—C7	−177.2 (5)	C23—C24—C25—C26	−178.5 (5)
C2—C1—C6—C5	−1.7 (8)	C21—C20—C25—C24	0.3 (8)
P1—C1—C6—C5	179.8 (4)	P2—C20—C25—C24	−174.6 (4)
C2—C1—C6—C7	176.3 (5)	C21—C20—C25—C26	177.9 (5)
P1—C1—C6—C7	−2.2 (7)	P2—C20—C25—C26	3.0 (8)
C5—C6—C7—O1	178.1 (5)	C24—C25—C26—O2	177.2 (6)
C1—C6—C7—O1	0.1 (9)	C20—C25—C26—O2	−0.5 (9)
C14—P1—C8—C9	124.1 (4)	C33—P2—C27—C28	−51.3 (5)
C1—P1—C8—C9	−124.0 (4)	C20—P2—C27—C28	62.3 (5)
Au1—P1—C8—C9	−1.1 (5)	Au2—P2—C27—C28	−173.9 (4)
C14—P1—C8—C13	−50.0 (5)	C33—P2—C27—C32	124.5 (4)
C1—P1—C8—C13	61.8 (5)	C20—P2—C27—C32	−121.8 (4)
Au1—P1—C8—C13	−175.2 (4)	Au2—P2—C27—C32	1.9 (5)
C13—C8—C9—C10	0.9 (8)	C32—C27—C28—C29	1.1 (8)
P1—C8—C9—C10	−173.2 (4)	P2—C27—C28—C29	176.9 (4)
C8—C9—C10—C11	−0.2 (9)	C27—C28—C29—C30	−1.4 (8)
C9—C10—C11—C12	−0.8 (9)	C28—C29—C30—C31	0.0 (9)
C10—C11—C12—C13	1.1 (9)	C29—C30—C31—C32	1.9 (9)
C9—C8—C13—C12	−0.7 (8)	C30—C31—C32—C27	−2.2 (8)
P1—C8—C13—C12	173.3 (4)	C28—C27—C32—C31	0.8 (8)
C11—C12—C13—C8	−0.3 (8)	P2—C27—C32—C31	−175.2 (4)
C1—P1—C14—C19	−14.6 (5)	C27—P2—C33—C38	−78.4 (5)
C8—P1—C14—C19	97.6 (5)	C20—P2—C33—C38	170.6 (4)
Au1—P1—C14—C19	−141.4 (4)	Au2—P2—C33—C38	42.6 (5)
C1—P1—C14—C15	168.4 (4)	C27—P2—C33—C34	96.8 (5)
C8—P1—C14—C15	−79.5 (5)	C20—P2—C33—C34	−14.2 (6)
Au1—P1—C14—C15	41.5 (5)	Au2—P2—C33—C34	−142.2 (4)
C19—C14—C15—C16	0.7 (8)	C38—C33—C34—C35	−1.9 (9)

P1—C14—C15—C16	177.9 (5)	P2—C33—C34—C35	−176.9 (5)
C14—C15—C16—C17	0.6 (9)	C33—C34—C35—C36	1.6 (9)
C15—C16—C17—C18	−1.0 (9)	C34—C35—C36—C37	0.0 (9)
C16—C17—C18—C19	0.0 (9)	C35—C36—C37—C38	−1.5 (9)
C15—C14—C19—C18	−1.7 (8)	C36—C37—C38—C33	1.2 (9)
P1—C14—C19—C18	−178.7 (4)	C34—C33—C38—C37	0.5 (8)
C17—C18—C19—C14	1.3 (8)	P2—C33—C38—C37	175.9 (4)