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## Key indicators

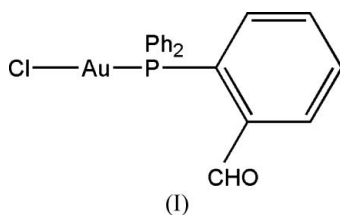
Single-crystal X-ray study  
T = 120 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$   
R factor = 0.037  
wR factor = 0.100  
Data-to-parameter ratio = 18.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.[2-(Diphenylphosphino- $\kappa P$ )benzaldehyde]gold(I) chloride

The title compound,  $[\text{AuCl}\{(2-(\text{C}_6\text{H}_5)_2\text{PC}_6\text{H}_4\text{CHO})\}]$ , 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  $\text{ClAu}(2\text{-Ph}_2\text{PC}_6\text{H}_4\text{X})$  ( $X = \text{H}, \text{OSiMe}_3$  or  $\text{OH}$ ) reveals that the nature of the *ortho* X substituent has a negligible effect on these structural parameters.

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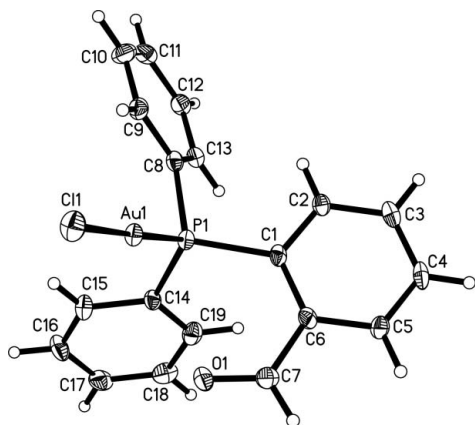
## Comment

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- $\text{Ph}_2\text{PC}_6\text{H}_4\text{CHO}$  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- $\text{Ph}_2\text{PC}_6\text{H}_4\text{CHO}$  have been reported (Yeh *et al.*, 2006).



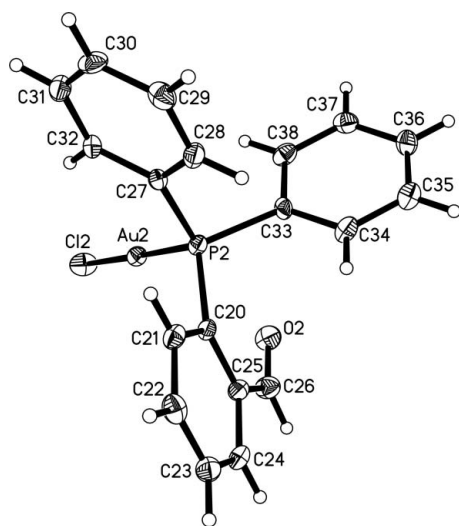
Compound (I),  $\text{ClAu}[2-(\text{C}_6\text{H}_5)_2\text{PC}_6\text{H}_4\text{CHO}]$ , crystallizes in a centrosymmetric space group, the asymmetric unit containing two independent molecules (Figs. 1 and 2, Table 1). The crystal structure of (I) confirms an essentially linear arrangement of both chloride and tertiary phosphine ligands around the gold(I) metal centre. In (I), the Au—P and Au—Cl bond lengths for both independent molecules 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- $\text{Ph}_2\text{PC}_6\text{H}_4\text{CHO}$ , 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 auriphilicity. 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<sub>2</sub>PC<sub>6</sub>H<sub>4</sub>CHO 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<sub>2</sub>Cl<sub>2</sub> (10 ml) solution of AuCl(tht) (tht is tetrahydrothiophene; 0.048 g,

0.150 mmol) was added 2-Ph<sub>2</sub>PC<sub>6</sub>H<sub>4</sub>CHO (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: <sup>31</sup>P{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, δ, p.p.m.): 32.2; <sup>1</sup>H NMR (CDCl<sub>3</sub>, δ, p.p.m.): 10.26 (CHO), 8.10–6.94 (arom. H); FT-IR (ν, cm<sup>-1</sup>): 1698 (CO), 1678 (CO), 333 (AuCl). Analysis, found: C 43.89, H 2.62%; C<sub>19</sub>H<sub>15</sub>AuClOP requires: C 43.65, H 2.90%. Colourless block crystals of (I) were obtained by vapour diffusion of diethyl ether into a CDCl<sub>3</sub> solution.

## Crystal data

[AuCl(C<sub>19</sub>H<sub>15</sub>OP)]  
*M*<sub>r</sub> = 522.70  
 Triclinic, P $\bar{1}$   
*a* = 10.2431 (2) Å  
*b* = 10.4949 (2) Å  
*c* = 16.6533 (3) Å  
 $\alpha$  = 97.1857 (7)°  
 $\beta$  = 103.5519 (9)°  
 $\gamma$  = 101.4375 (9)°

*V* = 1677.96 (6) Å<sup>3</sup>  
*Z* = 4  
*D*<sub>x</sub> = 2.069 Mg m<sup>-3</sup>  
 Mo K $\alpha$  radiation  
 $\mu$  = 9.02 mm<sup>-1</sup>  
*T* = 120 (2) K  
 Plate, colourless  
 0.25 × 0.20 × 0.04 mm

## Data collection

Bruker Nonius KappaCCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan using multiple and symmetry-related data measurements

(SORTAV; Blessing, 1995)  
*T*<sub>min</sub> = 0.128, *T*<sub>max</sub> = 0.697  
 29712 measured reflections  
 7704 independent reflections  
 6936 reflections with *I* > 2σ(*I*)  
*R*<sub>int</sub> = 0.063  
 $\theta$ <sub>max</sub> = 27.7°

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.037  
*wR* (*F*<sup>2</sup>) = 0.100  
*S* = 1.06  
 7704 reflections  
 415 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 5.6P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 3.10 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -1.40 \text{ e } \text{Å}^{-3}$

**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<sub>2</sub>PC<sub>6</sub>H<sub>4</sub>X) [X = H (Baenziger *et al.*, 1976), OSiMe<sub>3</sub> or OH (Hollatz *et al.*, 1999)].

	X = H	X = OH	X = OSiMe <sub>3</sub>
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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . 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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