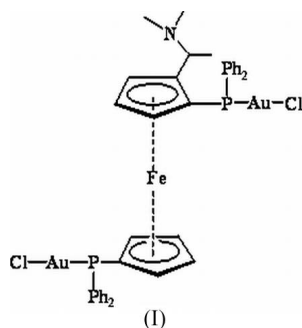


**{ $\mu$ -2-[1-(*N,N*-Dimethylamino)ethyl]ferrocene-1,1'-diylbis(diphenylphosphine)- $\kappa^2$ P:P'}-bis[chlorogold(I)]**Zolisa A. Sam,<sup>a</sup> Åke Oskarsson,<sup>b</sup>  
Sofi K. C. Elmroth<sup>c</sup> and  
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roodta.sci@mail.uovs.ac.za**Key indicators**Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma$ (C—C) = 0.015 Å  
*R* factor = 0.049  
*wR* factor = 0.109  
Data-to-parameter ratio = 19.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The structure of the title compound, [Au<sub>2</sub>Fe(C<sub>21</sub>H<sub>23</sub>NP)(C<sub>17</sub>H<sub>14</sub>P)Cl<sub>2</sub>], displays the pseudo-linear [P—Au—Cl = 175.4 (1) and 174.0 (1)°] two-coordinate geometry usually observed in gold(I) complexes. The Au—P bond distances are 2.237 (2) and 2.224 (2) Å and the Au—Cl distances are 2.271 (3) and 2.278 (2) Å. The bis(diphenylphosphino)ferrocenyl ligand links the gold metal centres in a bidentate fashion *via* the ferrocene group, thus leading to a binuclear gold system.

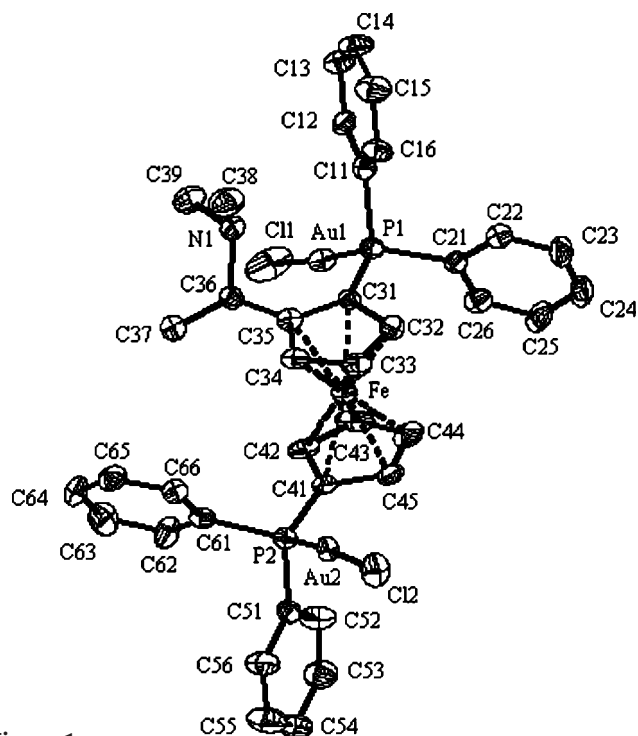
**Comment**

Research towards the synthesis and reactivity of transition metal complexes with ferrocene-bridged bis(tertiary phosphine) ligands such as 1,1'-bis(diphenylphosphino)ferrocene (dppf) has been increasingly interesting (Bruce *et al.*, 1990, Hor *et al.*, 1992). The use of these ferrocenylphosphines as ligands in coordination chemistry has enlarged the scope of metal complexes in the design of catalysts (Togni & Pastor, 1990), drugs (Hill *et al.*, 1989; Houlton *et al.*, 1991) and materials (Hayashi *et al.*, 1980). Catalytic reactions found in the literature include the gold(I)-catalysed aldol reactions of enolates with aldehydes to give optically active  $\beta$ -hydroxycarbonyl compounds (Ito *et al.*, 1986, 1987). Several chiral phosphine ligands have been employed in catalytic asymmetric reactions yielding high enantioselectivity. An example is the effect observed in the rhodium-catalysed asymmetric hydrogenation of  $\alpha$ -(acylamino)acrylic acids and/or their analogues leading to the hydrogenation products of over 90% *ee* (Morrison, 1985). However, few of them displayed this high enantioselectivity in other types of catalytic asymmetric reactions (Noyori & Takaya, 1990, and references therein). Reported in this paper is a modified bis(diphenylphosphino)ferrocenyl gold(I) analogue, (I), which has an ethylamine group specifically designed for improved solubility of the gold complex.

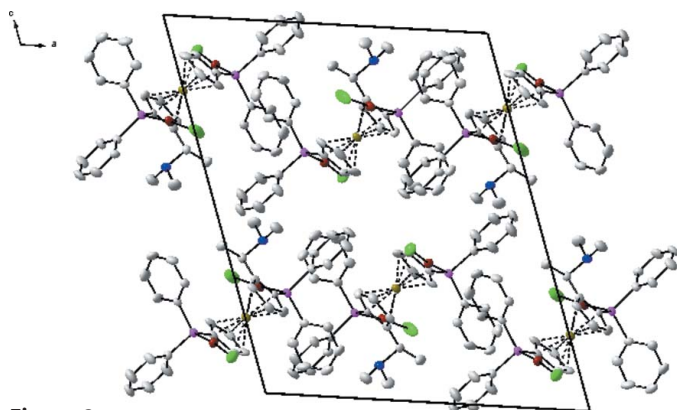


The compound is an Au<sup>I</sup> complex comprising a diphenylphosphine ferrocenyl ligand bearing phosphorus and nitrogen coordination sites. As gold is a soft metal, it preferentially

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**Figure 1**  
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.



**Figure 2**  
Packing diagram of (I). H atoms have been omitted for clarity.

bonds to the P atom, the soft coordination site in the ferrocenyl ligand. Since there are two of these sites in the complex, gold bonds to each site, leading to a binuclear gold system, as shown in Fig. 1.

The coordination mode of the bis(diphenylphosphine) moiety is of a *trans* open-bridging fashion, with the P1–Au1–Au2–P2 torsion angle = 178.8 (9)°. The angles between the approximately linear gold moieties and the corresponding cyclopentadienyl planes are 57.7 (2) and 70.8 (3)° for the P1–C11/Ring 3 and P2–C12/Ring 4 systems, respectively. The angle involving the two P atoms in the system (P···Fe···P) is 165.97 (7)°, and the cyclopentadienyl rings are partially eclipsed anticlinical relative to each other. The phenyl groups in the system are twisted approximately perpendicular to each other, with a  $(C_{ar}-P-C_{ar})_{av}$  of 104.6 (4)°. The coordination around the gold atoms is pseudo-linear (Table 1). The Au–P

and Au–Cl bond distances are within the normal range for (diphenylphosphino)ferrocenyl complexes found in the literature (Hill *et al.*, 1989; Crespo *et al.*, 2000; Canales *et al.*, 1997). For comparison, selected bond distances and angles for other similar Au<sup>I</sup> complexes are presented in Table 3.

The packing of the molecules in the unit cell is illustrated in Fig. 2. It is clear that the Fe atom lies very close to the *c* axis. The molecule was also investigated for possible  $\pi$ – $\pi$  interactions, but did not show any significant effects. However, weak intermolecular C–H···Cl hydrogen bonding is observed (Table 2).

## Experimental

The title compound was prepared according to a procedure similar to one described earlier by Gimeno *et al.* (1993). A solution of [(THT)AuCl] (THT = tetrahydrothiophene) (0.092 g, 0.3 mmol) in dichloromethane (30 ml) was treated with dppe-CH(CH<sub>3</sub>)N(CH<sub>3</sub>)<sub>2</sub> (Bjelosevic *et al.*, 2005) (0.094 g, 0.15 mmol) and the mixture was stirred for 30 min. The solution was concentrated to approximately 10 ml and addition of diethyl ether (25 ml) gave the desired product (0.15 g, 92%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz):  $\delta$  0.81 (*d*, 3H, CHCH<sub>3</sub>), 1.52 (*s*, 6H, NCH<sub>3</sub>), 3.74–4.91 (*m*, 8H), 7.34–7.74 (*m*, 20H, PC<sub>6</sub>H<sub>5</sub>) <sup>31</sup>P{<sup>1</sup>H} NMR (CDCl<sub>3</sub>, 121.5 MHz):  $\delta$  26.963 (*s*), 28.68 (*s*) IR (KBr,  $\nu$ , cm<sup>-1</sup>): 692 (*s*), 750 (*m*), 1023 (*w*), 1100 (*m*), 1434 (*s*), 1480 (*m*).

## Crystal data

[Au<sub>2</sub>Fe(C<sub>21</sub>H<sub>23</sub>NP)(C<sub>17</sub>H<sub>14</sub>P)Cl<sub>2</sub>]  
 $M_r = 1090.31$   
 Monoclinic,  $P2_1/n$   
 $a = 17.136$  (3) Å  
 $b = 10.946$  (2) Å  
 $c = 20.658$  (4) Å  
 $\beta = 108.39$  (3)°  
 $V = 3676.7$  (13) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.97$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 824 reflections  
 $\theta = 2.2$ – $21.3$ °  
 $\mu = 8.61$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Needle, orange  
 $0.17 \times 0.05 \times 0.03$  mm

## Data collection

Bruker SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1998)  
 $T_{min} = 0.600$ ,  $T_{max} = 0.772$   
 30273 measured reflections

8020 independent reflections  
 4488 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.098$   
 $\theta_{max} = 27.0$ °  
 $h = -21 \rightarrow 18$   
 $k = -13 \rightarrow 13$   
 $l = -26 \rightarrow 26$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.049$   
 $wR(F^2) = 0.109$   
 $S = 0.99$   
 8020 reflections  
 415 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.044P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 2.10$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.15$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Au1–P1	2.237 (2)	P1–C11	1.825 (9)
Au1–Cl1	2.271 (3)	P1–C21	1.839 (9)
Au2–P2	2.224 (2)	P2–C41	1.781 (9)
Au2–Cl2	2.278 (2)	P2–C51	1.826 (9)
P1–C31	1.810 (9)	P2–C61	1.828 (9)
P1–Au1–Cl1	175.4 (1)	C31–P1–Au1	117.1 (3)
P2–Au2–Cl2	174.0 (1)	C51–P2–C61	103.9 (4)
C11–P1–C21	105.3 (4)	C41–P2–Au2	113.3 (3)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C66-H66\cdots Cl1^i$	0.93	2.67	3.552 (10)	160

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

**Table 3**  
Comparative geometrical parameters (Å, °) for selected gold(I) ferrocenyl complexes.

Complex	Au-P	Au-Cl	P-Au-Cl
$[(dppf-R)(AuCl)_2]^a$	2.237 (2)	2.271 (3)	175.4 (1)
	2.224 (2)	2.278 (2)	174.0 (1)
$[(dppf)(AuCl)_2]^b$	2.2262 (13)	2.2815 (13)	179.59 (5)
$[(dppf)(AuCl_2)]^c$	2.239 (3)	2.300 (3)	176.0 (1)
	2.222 (3)	2.273 (4)	175.5 (1)
$[(dppf)(AuCl)_2]^d$	2.226 (1)	2.278 (1)	177.56 (8)
$[(C_{27}H_{28}FeNP)(AuCl)]^e$	2.24 (1)	2.32 (1)	176.5 (5)
$[(dppf-L)_2(AuCl)_3]^f$	2.31 (2)	2.52 (3)	113 (2)
	2.28 (2)	2.20 (2)	177 (2)

Notes: (a) this work,  $R = -CH(CH_3)N(CH_3)_2$ , dppf is 1,1'-bis(diphenylphosphino)ferrocene; (b) Canales *et al.* (1997), isolated as the  $CH_2Cl_2$  solvate; (c) Hill *et al.* (1989), isolated as the  $CH_3Cl$  solvate; (d) Canales *et al.* (1997); (e) Viotte *et al.* (1996), isolated as the  $C_6H_6$  1.5-solvate,  $C_{27}H_{28}FeNP = (\alpha\text{-dimethylamino}[3]\text{ferrocenophanyl})\text{diphenylphosphine}$ ; (f) Togni *et al.* (1990),  $L = -CH(CH_3)N(CH_3)CH_2CH_2N(CH_3)_2$ , isolated as the  $Et_2O$  solvate.

H atoms were positioned geometrically and allowed to ride on their parent atoms, with  $C-H = 0.93$  (aromatic),  $0.96$  (methyl) and  $0.98$  Å (methine), and  $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.5U_{eq}(\text{methyl } C)$ . The minimum and maximum residual electron density are located within  $1.2$  Å of the atom Au2, indicating no physical meaning.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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