C12	−0.0379 (7)	0.2284 (6)	0.6471 (4)	0.075 (2)
C13	−0.0166 (8)	0.2357 (7)	0.5755 (5)	0.098 (3)
C14	0.0427 (9)	0.1513 (10)	0.5406 (4)	0.105 (3)
C15	0.0800 (8)	0.0618 (8)	0.5771 (5)	0.091 (3)
C16	0.0583 (7)	0.0536 (6)	0.6478 (4)	0.071 (2)
C17	−0.0250 (6)	0.1252 (5)	0.7601 (3)	0.067 (2)
C21	0.0351 (7)	0.3763 (5)	0.8548 (4)	0.057 (2)
C22	−0.0418 (7)	0.4332 (5)	0.8057 (4)	0.070 (2)
C23	−0.1540 (7)	0.4894 (5)	0.8247 (4)	0.071 (2)
C24	−0.1927 (7)	0.4897 (6)	0.8929 (5)	0.084 (2)
C25	−0.1174 (7)	0.4343 (6)	0.9410 (4)	0.073 (2)
C26	−0.0056 (7)	0.3793 (5)	0.9230 (3)	0.064 (2)
C27	0.1531 (6)	0.3141 (5)	0.8333 (3)	0.065 (2)
C31	0.0565 (8)	−0.0277 (6)	0.9098 (3)	0.062 (2)
C32	0.1535 (8)	−0.1059 (7)	0.9181 (4)	0.082 (2)
C33	0.1331 (10)	−0.2151 (8)	0.9114 (5)	0.106 (3)
C34	0.0121 (12)	−0.2510 (7)	0.8964 (4)	0.101 (3)
C35	−0.0906 (9)	−0.1810 (8)	0.8884 (4)	0.099 (3)
C36	−0.0661 (8)	−0.0672 (7)	0.8949 (4)	0.083 (2)
C37	0.0887 (7)	0.0913 (5)	0.9140 (3)	0.076 (2)
C41	0.4154 (7)	0.1263 (5)	0.8197 (3)	0.056 (2)
C42	0.4730 (7)	0.0664 (6)	0.8743 (4)	0.078 (2)
C43	0.5905 (8)	0.0983 (9)	0.9053 (5)	0.106 (3)
C44	0.6533 (9)	0.1877 (10)	0.8848 (6)	0.120 (5)
C45	0.5991 (10)	0.2494 (8)	0.8305 (6)	0.118 (4)
C46	0.4808 (7)	0.2188 (6)	0.7987 (4)	0.078 (2)
C47	0.2874 (6)	0.0907 (5)	0.7852 (3)	0.065 (2)

Table 2. *Selected geometric parameters (Å, °)*

Ge—C17	1.974 (5)	C11—C17	1.500 (7)
Ge—C27	1.946 (6)	C21—C27	1.478 (7)
Ge—C37	1.956 (6)	C31—C37	1.486 (8)
Ge—C47	1.950 (6)	C41—C47	1.498 (8)
C17—Ge—C27	110.3 (3)	C37—Ge—C47	110.6 (3)
C17—Ge—C37	106.9 (3)	Ge—C17—C11	115.8 (4)
C17—Ge—C47	109.4 (2)	Ge—C27—C21	115.5 (4)
C27—Ge—C37	110.0 (3)	Ge—C37—C31	113.3 (4)
C27—Ge—C47	109.6 (3)	Ge—C47—C41	115.1 (4)
C12—C11—C17—Ge	−99.5 (6)	C32—C31—C37—Ge	91.4 (7)
C37—Ge—C17—C11	−162.6 (5)	C27—Ge—C37—C31	174.9 (5)
C22—C21—C27—Ge	−100.3 (6)	C42—C41—C47—Ge	93.5 (6)
C47—Ge—C27—C21	174.0 (5)	C17—Ge—C47—C41	168.2 (5)

Examination of the structure with *PLATON* (Spek, 1995*a*) showed that there were no solvent-accessible voids in the crystal lattice.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1992). Cell refinement: *CELDIM* and *SET4* (Enraf–Nonius, 1992). Data reduction: *DATRD2* in *NRCVAX94* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *NRCVAX94* and *SHELXL93* (Sheldrick, 1993). Molecular graphics: *NRCVAX94*, *ORTEPII* (Johnson, 1976) as implemented in *PLATON*, *PLUTON* (Spek 1995*b*). Software used to prepare material for publication: *NRCVAX94*, *SHELXL93*, *WordPerfect* (macro *PREPCIF*).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: AB1377). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Chloro[(α-dimethylamino[3]ferrocenophan-2-yl)diphenylphosphino]gold(I) Benzene Solvate

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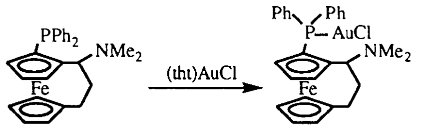
Abstract

The title complex, chloro{[1,1′-(1-dimethylamino-1,3-propanediyl)-2-ferrocenyl]diphenylphosphino-*P*}gold(I) 1.5-benzene solvate, [AuCl($C_{27}H_{28}$FeNP)].1.5C_6H_6, is the first gold(I) complex comprising a ferrocenophane ligand bearing phosphorus and nitrogen coordination sites. The Au atom is preferentially bound to the soft site, the P atom. The P, Au and Cl atoms are almost in a straight line and no interaction between the Au and N atoms is observed. There is little distortion of the *ansa* bridge and the conformation of the phenyl groups minimizes the steric contacts.

Comment

The importance attributed to phosphine–gold(I) complexes is undoubtedly related to their asymmetric catalysis properties and their antitumour activity. Moreover, some aminoferrocene derivatives (or their salts) also show cytostatic properties. But little is known about gold(I) complexes of amino–phosphino disubstituted ferrocenes (Hayashi, 1988; Ito, Sawamura, Kobayashi & Hayashi, 1988; Togni & Pastor, 1990). Recently, we published the structure of (1-phosphino-2-aminoferrocene)gold(I) (Viotte, Gautheron, Kubicki, Nifant'ev & Fricker, 1995) and here we report the structure of the first gold–ferrocenophane complex, chloro[(α-dimethylamino[3]ferrocenophanyl)-diphenylphosphino]gold(I) benzene solvate, (2).



(1) (2)

Several attempts were required for satisfactory collection of the X-ray data set. The high benzene content of the crystals led to decomposition even when the crystals were covered in lacquer and attempts at fixing the crystals in a tube near the mother liquor resulted in crystal movement. Nevertheless it was possible to measure X-ray reflections of good enough quality for a structure determination and refinement to be carried out.

The structure of (2) (Fig. 1) reveals that gold (a soft metal) is bonded to the P atom, the softer coordination site of the ferrocenyl ligand. The two cyclopentadienyl rings are planar, parallel and eclipsed. The range of the Fe to cyclopentadienyl C-atom distances [1.97 (4)–2.09 (5) Å] is similar to that for other ferrocenes (Hayashi, Yamamoto, Ito, Nishioka, Miura & Yanagi, 1989), but the two bridgehead C atoms are not symmetrically bonded to the Fe atom. The *ansa* bridge is slightly distorted with the central C atom nearest to being sp^3 hybridized. The C17—C18 bond is the best plane of the cyclopentadienyl ligand, whereas the C21—C20 bond is oriented out of the second pentahapto ring towards the Fe atom. The Au—P bond length [2.24 (1) Å] falls in the range of those observed for linear two-coordinate gold(I) complexes [2.22–2.24 Å; Attar, Bearden, Alcock, Alyea & Nelson, 1990], but the Au—Cl distance [2.32 (1) Å] is greater than the observed average [2.28 Å; Jones, Erdbrügger, Hohbein & Schwarzmann, 1988]. The P—Au—Cl angle is almost linear [176.5 (5)°] and is nearly the same as those observed in other two-coordinate gold(I) complexes (Jones *et al.*, 1988).

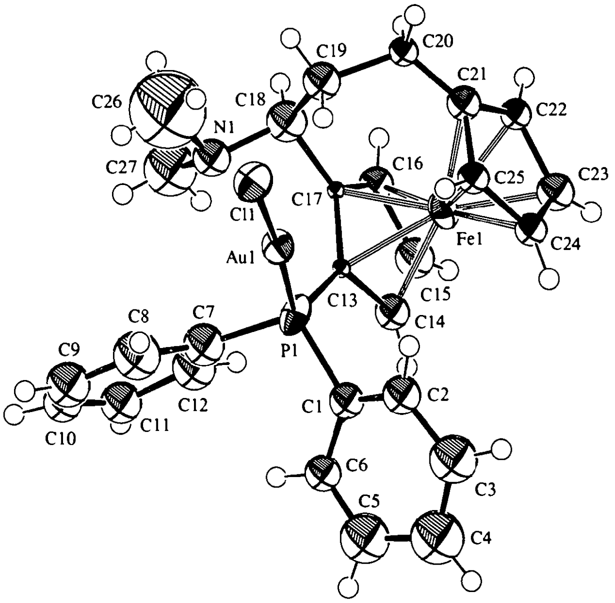


Fig. 1. The molecular structure of (2). The benzene solvent molecule has been omitted for clarity. Displacement ellipsoids are plotted at the 50% probability level.

The pyramidal environment of the N atom is distorted, with the pair of free electrons oriented towards the Au atom, but from the observed Au—N distance [3.57 (5) Å] there is no significant interaction between these two atoms. The pseudo-tetrahedral arrangement of the P atom is consistent with one P—$\mathrm{C_{phenyl}}$ distance being substantially shorter than the other bonds. The two phenyl rings are in a conformation which minimize the steric contacts, nevertheless, the C1–C6 phenyl ring is not planar because of the close proximity of the ferrocene moiety. The P—C1 and P—C7 bonds are approximately in the best plane of their corresponding phenyl groups, whereas the P atom deviates slightly from the cyclopentadienyl plane towards the Fe atom. There are benzene molecules of crystallization and one of these sits on a crystallographic inversion centre.

The gold reagent was obtained according to the method of Uson & Laguna (1986) and the ligand precursor was prepared according to the method described in the literature (Turbitt & Watts, 1972; Dixneuf, 1971; Marr & Hunt, 1969). For further reading on the crystallography of gold(I)–ferrocenyl derivatives see Baenziger, Bennett & Soboroff (1976), Harker & Tiekink (1991) and Muir, Cuadrado & Muir (1991). Related compounds which possess antitumour activity can be found in Köpf-Maier & Köpf (1986), Berners-Price *et al.* (1986, 1990) and Houlton, Roberts & Silver (1991).

The use of ferrocenyl compounds in asymmetric synthesis has been discussed by Ito, Sawamura & Hayashi (1986).

Experimental

The ligand (1), used for preparing the title compound, was synthesized by adaptation of the literature to the selective *ortho* lithiation of α-dimethylamino[3]ferrocenophane followed by reaction with $ClPPh_2$. The gold complex, (2), was obtained by reacting compound (1) with $[(tht)AuC_6F_5]$ (tht is tetrahydrothiophene) in dichloromethane at room temperature under a pure dry-argon atmosphere. Orange crystals suitable for X-ray measurements were grown from a benzene solution. Full elemental and NMR analyses of the products as well as Mössbauer data of the gold adduct confirmed the expected compositions.

Crystal data

$[AuCl(C_{27}H_{28}FeNP)].1.5C_6H_6$
$M_r = 802.94$
Monoclinic
$P2_1/c$
$a = 9.285\ (3)$ Å
$b = 18.287\ (8)$ Å
$c = 19.427\ (6)$ Å
$\beta = 99.55\ (4)^\circ$
$V = 3253\ (4)$ Å^3
$Z = 4$
$D_x = 1.639$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 8.5$–12.54°
$\mu = 5.1$ mm^{-1}
$T = 296$ K
Irregular
$0.30 \times 0.15 \times 0.15$ mm
Yellow

Data collection

Rigaku AFC-6*S* diffractometer
ω scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.88$, $T_{\max} = 1.00$
2274 measured reflections
2019 independent reflections

1057 observed reflections $[I > 3\sigma(I)]$
$R_{\rm int} = 0.042$
$\theta_{\max} = 40.0^\circ$
$h = 0 \rightarrow 6$
$k = 0 \rightarrow 17$
$l = -18 \rightarrow 18$
3 standard reflections monitored every 150 reflections intensity decay: 19%

Refinement

Refinement on F
$R = 0.068$
$wR = 0.064$
$S = 2.97$
921 reflections
185 parameters
H-atom parameters not refined
$w = 4F_o^2/\sigma^2(F_o^2)$

$(\Delta/\sigma)_{\max} = 0.1$
$\Delta\rho_{\max} = 0.86$ e Å^{-3}
$\Delta\rho_{\min} = -0.95$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$B_{\rm eq} = (1/3)\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
Au	0.4959 (2)	0.1685 (1)	0.6432 (1)	2.7 (1)
Fe	0.7915 (8)	0.3657 (4)	0.6867 (3)	2.9 (4)
Cl	0.369 (1)	0.0958 (8)	0.7106 (6)	4.3 (9)
P	0.610 (2)	0.2359 (9)	0.5725 (7)	3 (1)
N	0.352 (4)	0.346 (2)	0.598 (2)	3 (1)
C1	0.765 (6)	0.197 (3)	0.554 (3)	3 (1)
C2	0.842 (6)	0.169 (3)	0.604 (2)	3 (1)
C3	0.981 (6)	0.142 (3)	0.596 (3)	6 (2)
C4	1.029 (6)	0.133 (4)	0.528 (3)	7 (2)
C5	0.920	0.159 (4)	0.473 (3)	6 (2)
C6	0.795 (5)	0.191 (3)	0.486 (2)	3 (1)
C7	0.491 (6)	0.246 (3)	0.490 (3)	4 (1)
C8	0.377 (6)	0.198 (3)	0.463 (3)	5 (2)
C9	0.295 (5)	0.208 (3)	0.396 (3)	5 (1)
C10	0.321 (6)	0.266 (3)	0.354 (2)	4 (1)
C11	0.428 (6)	0.304 (3)	0.372 (2)	4 (1)
C12	0.511 (5)	0.295 (3)	0.446 (3)	5 (1)
C13	0.667 (4)	0.322 (3)	0.599 (2)	1 (1)
C14	0.803 (5)	0.359 (3)	0.580 (2)	3 (1)
C15	0.812 (6)	0.434 (3)	0.603 (2)	4 (1)
C16	0.680 (5)	0.450 (3)	0.632 (2)	3 (1)
C17	0.601 (5)	0.386 (3)	0.629 (2)	1 (1)
C18	0.450 (6)	0.382 (3)	0.656 (2)	4 (1)
C19	0.456 (5)	0.341 (3)	0.727 (2)	4 (1)
C20	0.572 (5)	0.373 (3)	0.785 (2)	2 (1)
C21	0.718 (6)	0.359 (3)	0.786 (2)	3 (1)
C22	0.829 (5)	0.412 (3)	0.786 (2)	2 (1)
C23	0.961 (5)	0.378 (3)	0.763 (3)	3 (1)
C24	0.933 (5)	0.299 (3)	0.752 (2)	3 (1)
C25	0.786 (5)	0.288 (3)	0.763 (2)	2 (1)
C26	0.224 (10)	0.319 (5)	0.621 (4)	15 (2)
C27	0.312 (6)	0.404 (3)	0.539 (3)	7 (2)
C28	1.023 (7)	0.093 (4)	0.795 (3)	9 (2)
C29	1.015 (7)	0.120 (4)	0.863 (3)	8 (2)
C30	0.886 (8)	0.114 (4)	0.892 (3)	7 (2)
C31	0.760 (7)	0.081 (4)	0.851 (3)	8 (2)
C32	0.776 (8)	0.063 (4)	0.785 (4)	8 (2)
C33	0.898 (8)	0.058 (3)	0.765 (3)	5 (2)
C34	0.567 (8)	−0.000 (4)	0.576 (3)	7 (2)
C35	0.646 (6)	0.009 (3)	0.524 (3)	6 (2)
C36	0.578 (8)	0.007 (4)	0.454 (4)	8 (2)

Table 2. *Selected geometric parameters (Å, °)*

Au—N	3.57 (5)	N—C26	1.43 (8)
Au—Cl	2.32 (1)	N—C27	1.55 (6)
Au—P	2.24 (1)	C17—C18	1.57 (6)
P—C1	1.69 (5)	C18—C19	1.56 (6)
P—C7	1.79 (5)	C19—C20	1.54 (5)
P—C13	1.71 (5)	C20—C21	1.37 (5)
N—C18	1.49 (5)		
Cl—Au—P	176.5 (5)	N—C18—C19	112 (4)
Au—P—C13	118 (2)	C18—N—C26	111 (5)
Au—P—C1	114 (2)	C18—N—C27	107 (4)
Au—P—C7	109 (2)	C26—N—C27	111 (5)
P—C13—C17	136 (4)	C17—C18—C19	114 (4)
C13—C17—C18	123 (5)	C18—C19—C20	112 (4)
N—C18—C17	104 (4)	C19—C20—C21	120 (5)

A scan rate of 8.0° min^{-1} (in ω) and a scan width of $(1.01 + 0.30\tan\theta)^\circ$ were used. The structure was solved by direct methods (*SHELXS*86; Sheldrick, 1985) and refined either anisotropically or isotropically. H atoms were included in the structure-factor calculation in idealized positions and fixed with isotropic displacement parameters. Neutral atom-scattering factors were taken from Cromer & Waber (1974). All calculations were performed using the *TEXSAN* (Molecular Structure Corporation, 1985) crystallographic software package.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: PA1217). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Aqua(L-*O*-serine phosphato)calcium(II)

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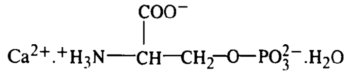
Abstract

In the crystal structure of the title compound, $[Ca(C_3H_6NO_6P)(H_2O)]$, the Ca ion is bonded to six O atoms, three from the phosphate group, two from the carboxyl group and one from the water molecule. The coordination geometry around the Ca ion is distorted octahedral. The L-*O*-serine phosphate molecules are connected in a three-dimensional manner through O—Ca—O bonds. The structural parameters also suggest the presence of intermolecular N—H···O hydrogen bonds.

Comment

Phosphorylated proteins have various important physiological functions in many hormonal regulatory systems, muscle, cells and organs (Taborsky, 1974; Rubin & Rosen, 1975; Cohen, 1982; Martin, Mayes & Rodwell, 1983). In some cases, the function of phosphoproteins has been explained in relation to their Ca-ion binding ability. In muscle, the calmodulin-mediated phosphorylation of light chains of muscle myosin begins the attachment–detachment contraction cycle of smooth muscle. It has been proposed that the phosphate on the myosin light chains may chelate with Ca ions. In milk, dephosphorylation of casein micelles containing Ca ions by phosphoprotein phosphatase causes extensive degradation of the micelles. In bones and/or teeth, phosphopeptide-bound collagen and/or phosphoryn bind Ca ions strongly. For these reasons, it is important to elucidate structurally the interaction between phosphoproteins and metal ions, especially Ca ions. We report here the structural features of the chelate compound of L-*O*-serine phosphate and the Ca ion, (I), as a useful model of the interaction of phosphoproteins with the Ca ion.



$$\mathrm{Ca^{2+}.{}^{+}H_3N{-}\overset{\displaystyle COO^-}{\overset{|}{CH}}{-}CH_2{-}O{-}PO_3^{2-}.H_2O}$$

(I)

The crystal structures of L-serine phosphate (McCallum, Robertson & Sim, 1959) and DL-*O*-serine phosphate monohydrate (Putkey & Sundaralingam, 1970) have been reported previously. Fig. 1 shows the molecular structure and atom-numbering scheme of