Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Chloro[(di-*tert*-butylphosphino)cobaltocenium-*κP*]gold(I) hexafluorophosphate

Li-Yan Li, Yong Ren, Guang-Ao Yu* and Sheng-Hua Liu

Key Laboratory of Pesticides and Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail:
yuguang@mail.ccnu.edu.cn

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.014 Å
R factor = 0.043
wR factor = 0.111
Data-to-parameter ratio = 16.1

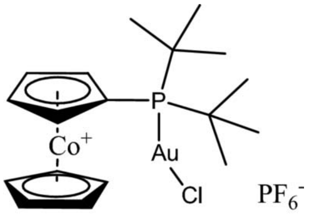
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 16 December 2005
Accepted 3 January 2006

In the crystal structure of the title compound, [AuCl{Co(C_5H_5)($C_5H_4P^tBu_2$)}]PF_6 or [AuCo(C_5H_5)($C_{13}H_{22}P$)Cl]PF_6, hexafluorophosphate is an uncoordinated anion. The structure contains η^5-(C_5H_5)C—H···F hydrogen bonds.

Comment

The synthesis and reactivity of transition metal complexes with ferrocene-bridged bis(tertiary phosphine) ligands such as 1,1′-bis(diphenylphosphino)ferrocene (dppf) have been a topic of interest in the last few years, mainly because of the catalytic properties displayed by some of them (Cullen *et al.*, 1982). Moreover, the antitumor activity of bis(diphenylphosphines) and their bis(gold(I)) complexes has been of recent interest (Mirabelli *et al.*, 1987). We have studied the coordination of cobaltocenylphosphine as a bridging or chelating ligand in two-coordinate gold(I) complexes.



(I)

In the title compound, (I), the Co1—C bond distances for the η^5-(C_5H_4) ring range from 2.001 (9) to 2.066 (7) Å, similar to the η^5-(C_5H_5) ring which has a range of 2.000 (9)–2.062 (10) Å. The Co1···*Cg*1 and Co1···*Cg*2 distances (*Cg*1 and *Cg*2 are the centroids of the η^5-(C_5H_4) and η^5-(C_5H_5) rings, respectively) are 1.643 (5) and 1.638 (4) Å, respectively. The cyclopentadienyl C—C bond distances for the η^5-(C_5H_5) and η^5-(C_5H_4) rings are in the ranges 1.370 (15)–1.416 (18) Å and 1.382 (15)–1.434 (10) Å, respectively. The P1—C10 bond distance is significantly shorter than the P1—C11 and P1—C15 distances (Table 1).

The dihedral angle between the two cyclopentadienyl rings is 9.2 (7)°. Analysis of the hydrogen bonding in the title compound shows weak C—H···F interactions (Fig. 2 and Table 2).

Experimental

The title compound was synthesized following a standard procedure (Al-sa'ady *et al.*, 1985). Crystals suitable for data collection were obtained by slow diffusion of hexane into a dichloromethane solution at room temperature.

Crystal data

$[AuCo(C_5H_5)(C_{13}H_{22}P)Cl]PF_6$
$M_r = 710.68$
Triclinic, $P\overline{1}$
$a = 8.4139$ (12) Å
$b = 9.3680$ (13) Å
$c = 15.031$ (2) Å
$\alpha = 100.384$ (2)°
$\beta = 99.487$ (2)°
$\gamma = 102.035$ (2)°
$V = 1114.3$ (3) Å^3
$Z = 2$
$D_x = 2.118$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5047 reflections
$\theta = 2.2$–25.9°
$\mu = 7.64$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
8158 measured reflections
4303 independent reflections
3888 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.085$
$\theta_{\rm max} = 26.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 10$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.111$
$S = 1.12$
4303 reflections
268 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 2.53P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 1.98$ e Å^{-3}
$\Delta\rho_{\rm min} = -1.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Au1—P1	2.2449 (18)	C11—P1	1.874 (8)
Au1—Cl1	2.294 (2)	C15—P1	1.881 (8)
C10—P1	1.834 (7)		
P1—Au1—Cl1	173.69 (7)	C10—P1—Au1	106.2 (2)
C10—P1—C11	108.3 (3)	C11—P1—Au1	112.6 (3)
C10—P1—C15	103.5 (4)	C15—P1—Au1	111.8 (3)
C11—P1—C15	113.7 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F6$^{\rm i}$	0.98	2.54	3.46 (2)	157
C7—H7···F5$^{\rm i}$	0.98	2.46	3.225 (14)	135
C4—H4···F3$^{\rm ii}$	0.98	2.39	3.194 (14)	139
C8—H8···F4$^{\rm ii}$	0.98	2.39	3.288 (15)	151
C6—H6···F3$^{\rm iii}$	0.98	2.39	3.259 (12)	148
C9—H9···F1$^{\rm iv}$	0.98	2.47	3.141 (11)	125

Symmetry codes: (i) $x+1, y+1, z$; (ii) $-x+2, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+2$; (iv) $x+1, y, z$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H(methyl H) = 0.98 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$, C—H(cyclopentadienyl H) = 0.98 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The largest peak in the difference map is 0.84 Å from atom Au1 and the deepest hole is 1.23 Å from P1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

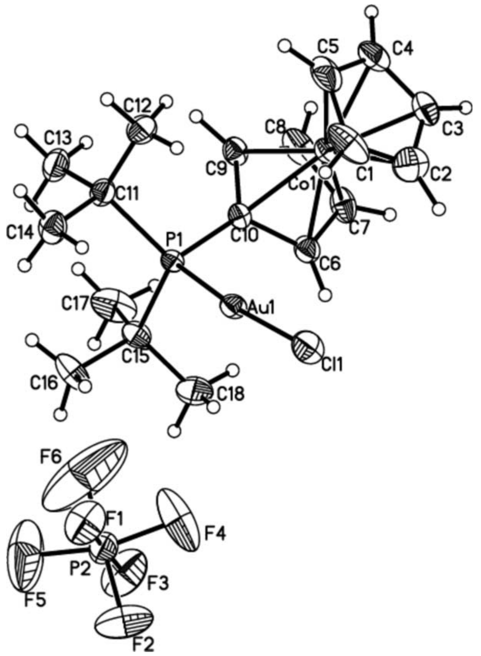


Figure 1
The constituent ions of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probablity level.

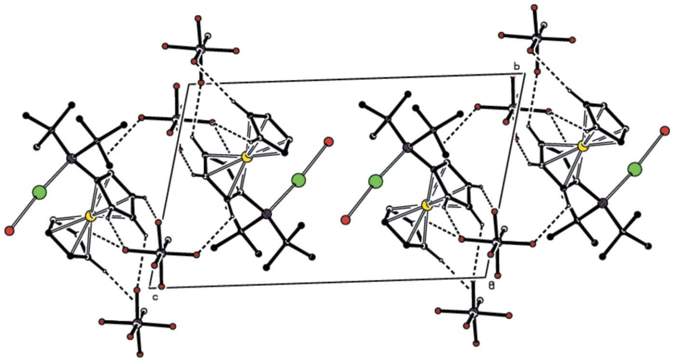


Figure 2
The packing of (I), showing the C—H···F hydrogen bonds as dashed lines. H atoms not involved in these hydrogen bonds have been omitted.

The authors acknowledge financial support from the National Natural Science Foundation of China (No. 20572029), New Century Excellent Talents in Universities (NCET-04-0743), the Program for Excellent Research Groups of Hubei Province (No. 2004ABC002) and the Natural Science Foundation of Hubei Province (No. 2005ABA038).

References

Al-sa'ady, A. K., McAuliffe, C. A., Parish, R. V. & Sandbank, J. A. (1985). *Inorg. Synth.* **23**, 191–194.
Bruker(2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Cullen, W. R., Woollins, J. D. (1982). *Coord. Chem. Rev.* **39**, 1–30.
Mirabelli, C. K., Hill, D. T., Faucette, L. F., McCabe, F. L., Girard, G. R., Bryan, D. B., Sutton, B. M., Bartus, J. O., Crooke, S. T. & Johnson, R. K. (1987). *J. Med. Chem.* **30**, 2181–2190.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

m250 Li *et al.* • $[AuCo(C_5H_5)(C_{13}H_{22}P)Cl]PF_6$ *Acta Cryst.* (2006). E**62**, m249–m250