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[1,1′-Bis(diphenylphosphino)ferrocene-$\kappa^2 P,P'$]-dichloroplatinum(II) chloroform solvate

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Key indicators

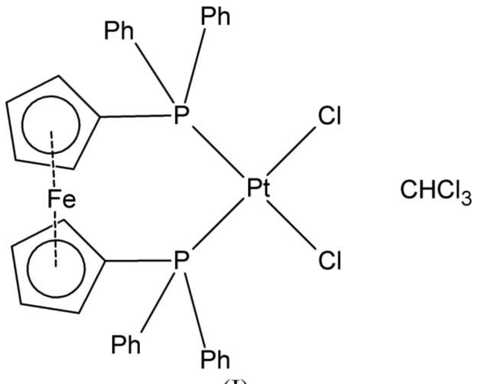
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.004 Å
R factor = 0.022
wR factor = 0.052
Data-to-parameter ratio = 20.7

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

The title compound, $[PtCl_2\{P(C_6H_5)_2Fe(C_5H_4)_2P(C_6H_5)_2\}]\cdot CHCl_3$, crystallizes with an accompanying chloroform solvent molecule. The Pt atom shows square-planar coordination.

Comment

Ferrocenylphosphines have found useful synthetic application as ligands in the rhodium-, ruthenium- and palladium-catalyzed hydrogenation of olefins (Cullen & Woollins, 1982) and the nickel- and palladium-catalyzed Grignard cross-coupling reactions (Hayashi, Konishi, Fukushima *et al.*, 1982; Hayashi, Konishi, Ito & Kumada, 1982; Hayashi *et al.*, 1984).



(I)

The title compound, (I), crystallizes with a chloroform solvent molecule (Fig. 1). It shows a slightly distorted coordination environment for the Pt centre, which is displaced 0.0502 (3) Å from the plane formed by the four coordinating atoms (r.m.s. deviation of fitted atoms = 0.048 Å).

Usually, ferrocenyl fragments possess geometric parameters similar to those of ferrocene and its derivatives [Cambridge Structural Database (CSD), Version 5.27, August 2006 update; Allen, 2002]. In the present example, the cyclopentadienyl rings (Cp) are nearly planar (r.m.s. deviation of fitted atoms in Cp rings = 0.0051 and 0.0039 Å for rings C31—C35 and C41—C45, respectively) with an interplanar angle of 4.6 (2)°. Furthermore, the Cp rings have a staggered conformation due to coordination to the Pt centre.

Other related compounds have also been reported. These include structures with a different solvent (Clemente *et al.*, 1986) and also without an accompanying solvent (de Lima *et al.*, 1995). An overlay (Fig. 2) of these structures with (I) shows the compound to be fairly rigid, with the most notable variations on the periphery of the molecule, possibly due to packing effects. The palladium congener, containing a chloroform solvate, has been reported by several authors (Hayashi *et al.*, 1984; Xi *et al.*, 1991); it shows isomorphism with the title compound. Two additional Pd congeners (with dichloromethane solvate) are also reported in the space group $P2_1/c$ (Butler *et al.*, 1985; de Lima *et al.*, 1995).

Experimental

Dichloro(1,5-cyclooctadiene)platinum(II) was prepared using the method described previously by Clark & Manzer (1973), while the other chemicals were obtained from Sigma–Aldrich. The title compound was synthesized from equimolar amounts (*ca* 1 mmol) of dichloro(1,5-cyclooctadiene)platinum(II) and 1,1′-bis(diphenylphosphino)ferrocene in chloroform (10 ml). Suitable crystals were obtained by slow evaporation of the reaction mixture.

Crystal data

$[PtFeCl_2(C_{17}H_{14}P)_2]\cdot CHCl_3$
$M_r = 939.71$
Monoclinic, $P2_1/n$
$a = 12.1534\ (6)$ Å
$b = 16.4121\ (8)$ Å
$c = 16.7053\ (8)$ Å
$\beta = 94.394\ (3)^\circ$
$V = 3322.3\ (3)$ Å^3
$Z = 4$
$D_x = 1.879$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 5.17$ mm^{-1}
$T = 100\ (2)$ K
Cuboid, yellow
0.29 × 0.17 × 0.11 mm

Data collection

Bruker X8 APEXII diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*, Bruker, 2004)
$T_{min} = 0.316$, $T_{max} = 0.600$ (expected range = 0.298–0.566)
38208 measured reflections
8237 independent reflections
7233 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 28.3^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.052$
$S = 1.06$
8237 reflections
397 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 1.9034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.99$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt—P1	2.2549 (7)	Pt—Cl1	2.3517 (6)
Pt—P2	2.2699 (7)	Pt—Cl2	2.3562 (6)
P1—Pt—P2	99.34 (2)	P1—Pt—Cl2	90.05 (2)
P1—Pt—Cl1	176.11 (2)	P2—Pt—Cl2	169.41 (2)
P2—Pt—Cl1	84.54 (2)	Cl1—Pt—Cl2	86.06 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C66—H66···Cl1	0.95	2.72	3.350 (3)	124

Aromatic and methine H atoms were placed in geometrically idealized positions, with C—H = 0.93–0.98 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

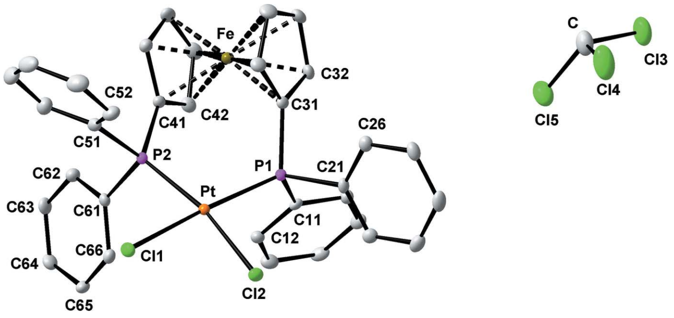


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity. For the C atoms, the first digit indicates the ring number and the second digit indicates the position of the atom in the ring.

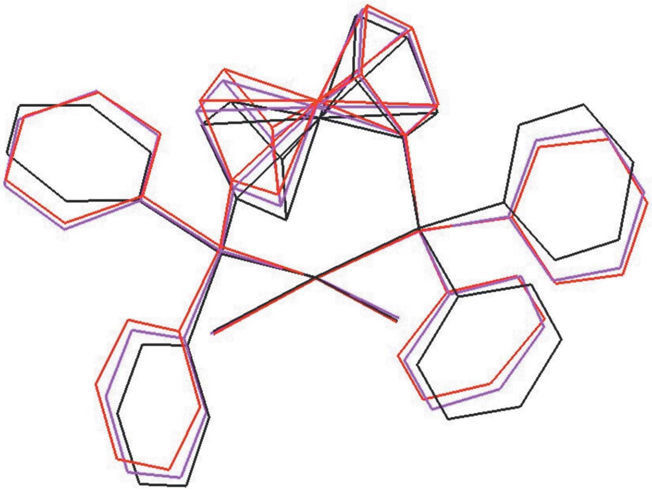


Figure 2
Superimposed line drawings of the compounds reported by Clemente *et al.* (1986) and de Lima *et al.* (1995) with the title compound, in violet, red and black, respectively. H atoms and solvent molecules have been omitted.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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