

$(\eta^5\text{-Cyclopentadienyl})(\eta^6\text{-1,2-dichlorobenzene})\text{iron(II) hexafluorophosphate}$

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Key indicators

Single-crystal X-ray study

 $T = 150\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$ R factor = 0.041 wR factor = 0.108

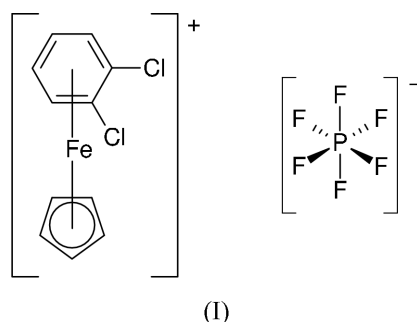
Data-to-parameter ratio = 25.2

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

At 150 K, the iron(II) sandwich complex cation of the salt $[\text{Fe}(\eta^5\text{-C}_5\text{H}_5)(\eta^6\text{-C}_6\text{H}_4\text{Cl}_2)]\text{PF}_6$ has almost parallel rings and the two C—Cl bonds of the 1,2-dichlorobenzene ligand are bent slightly towards the iron centre.

Comment

The title compound, (I), is a well known organometallic synthon (Piorko & Sutherland, 1997) and has previously only been structurally characterized in a series of host–guest complexes (Holman *et al.*, 1997).



The C atoms of each of the two aromatic ligands are nearly perfectly coplanar and the two least-squares planes are almost parallel; the angle between the normals to these is $178.68(9)^\circ$. The Fe atom lies $1.6686(3)\text{ \AA}$ from the least-squares plane of the cyclopentadienyl ligand, with an average Fe1—C distance of $2.053(4)\text{ \AA}$, and $1.5304(3)\text{ \AA}$ from the least-squares plane of the 1,2-dichlorobenzene ligand, with an average Fe1—C distance of $2.079(3)\text{ \AA}$. The two C—Cl bonds are distorted slightly towards the iron centre, lying respectively $0.0297(6)$ and $0.0572(6)\text{ \AA}$ out of the least-squares plane of the benzene ring.

Experimental

The title compound was prepared according to the method of Piorko & Sutherland (1997). Suitable crystals were grown from ethanol/dichloromethane by slow evaporation.

Crystal data

 $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_6\text{H}_4\text{Cl}_2)]\text{PF}_6$ $M_r = 412.90$ Monoclinic, $P2_1/c$ $a = 7.8972(6)\text{ \AA}$ $b = 12.4909(7)\text{ \AA}$ $c = 13.8701(11)\text{ \AA}$ $\beta = 92.325(6)^\circ$ $V = 1367.06(17)\text{ \AA}^3$ $Z = 4$ $D_x = 2.006\text{ Mg m}^{-3}$ Mo $K\alpha$ radiation

Cell parameters from 21436

reflections

 $\theta = 2.2\text{--}32.3^\circ$ $\mu = 1.67\text{ mm}^{-1}$ $T = 150(2)\text{ K}$

Fragment, orange

 $0.45 \times 0.30 \times 0.25\text{ mm}$

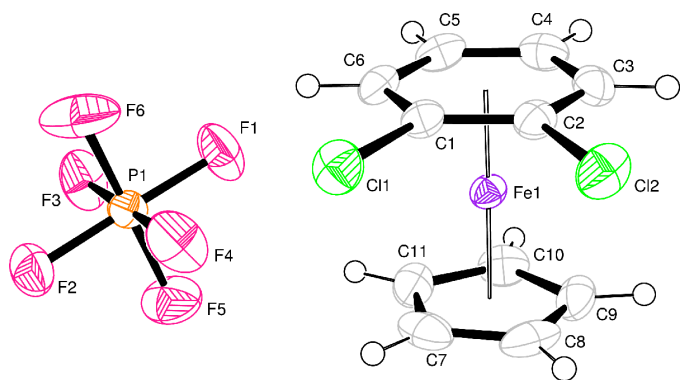


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

Data collection

Stoe IPDS-II diffractometer
Area-detector scans
Absorption correction: numerical
(*X-SHAPE*; Stoe & Cie, 2001)
 $T_{\min} = 0.594$, $T_{\max} = 0.834$
25 607 measured reflections
4814 independent reflections

3448 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\text{max}} = 32.3^\circ$
 $h = -11 \rightarrow 11$
 $k = -18 \rightarrow 17$
 $l = -20 \rightarrow 17$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.109$
 $S = 1.03$
4814 reflections
191 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.64 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.63 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0084 (10)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Fe1—C7	2.042 (3)	Cl2—C2	1.723 (2)
Fe1—C11	2.047 (2)	C1—C2	1.411 (3)
Fe1—C8	2.048 (2)	C1—C6	1.413 (3)
Fe1—C10	2.062 (2)	C6—C5	1.405 (3)
Fe1—C9	2.066 (2)	C4—C5	1.405 (4)
Fe1—C3	2.070 (2)	C4—C3	1.408 (3)
Fe1—C2	2.075 (2)	C3—C2	1.399 (3)
Fe1—C6	2.078 (2)	C9—C8	1.391 (4)
Fe1—C5	2.078 (2)	C9—C10	1.420 (3)
Fe1—C4	2.084 (2)	C10—C11	1.412 (4)
Fe1—C1	2.088 (2)	C7—C11	1.402 (4)
Cl1—C1	1.718 (2)	C7—C8	1.404 (4)
C2—C1—C11	121.20 (16)	C3—C2—Cl2	119.12 (16)
C6—C1—C11	119.27 (16)	C1—C2—Cl2	120.31 (17)

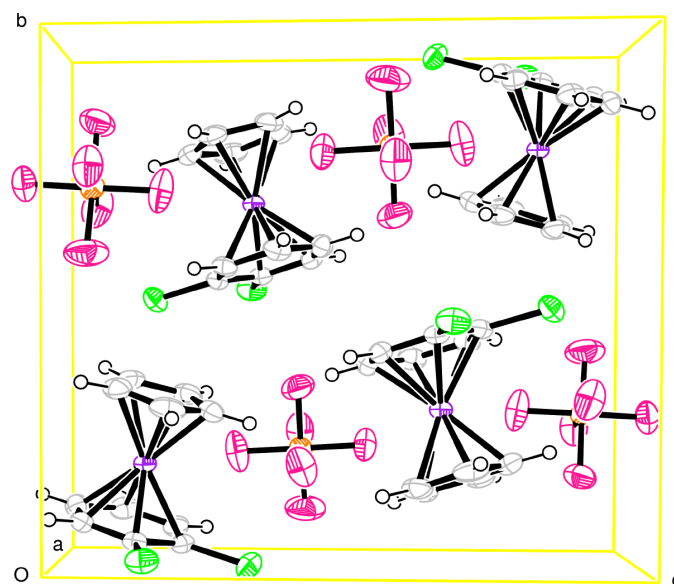


Figure 2
The molecular packing of (I), viewed normal to (100).

All H atoms were initially located in a difference Fourier map, then placed in geometrically idealized positions with C—H distances of 0.95 \AA and $U_{\text{iso}}(\text{H})$ values set at $1.2U_{\text{eq}}(\text{C})$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *X-STEP32* (Stoe & Cie, 2001) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *WinGX* (Farrugia, 1999) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX*.

References

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