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Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
Disorder in solvent or counterion
 R factor = 0.046
 wR factor = 0.129
Data-to-parameter ratio = 14.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>. $(\eta^5\text{-Cyclopentadienyl})[\eta^5\text{-1-(diphenyl-
phosphino)cyclopentadienyl}]$ cobalt(III)
hexafluorophosphateIn the title cobaltocenium compound, $[\text{Co}(\text{C}_5\text{H}_5)(\text{C}_{17}\text{H}_{14}\text{P})]\text{-PF}_6$, the Co^{III} atom carries both cyclopentadienyl and diphenylphosphinocyclopentadienyl ligands inclined to each other at 3.2 (1°). The disordered PF_6^- anion links with the cobaltocenium cation *via* weak $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds.Received 6 December 2005
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Comment

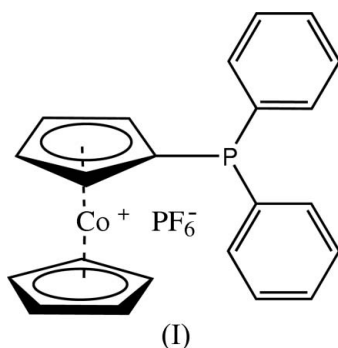
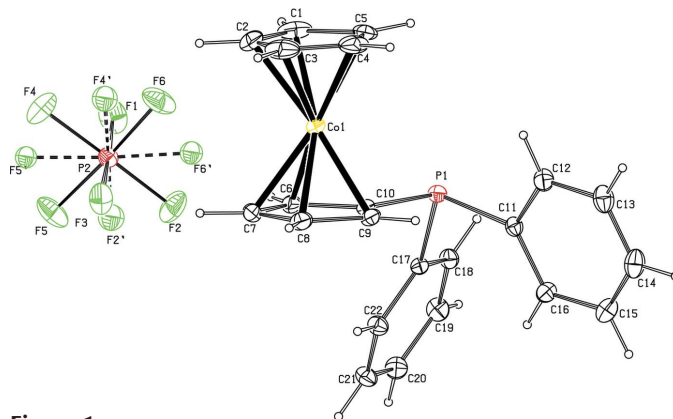
Cobaltocene derivatives have been applied as catalysts in cross-coupling reactions (Mathews *et al.*, 2000). As part of our investigations of new catalysts, we have focused our attention on cobaltocenium compounds and report here the structure of the title compound, (I) (Fig. 1 and Table 1).In (I), the Co^{III} atom carries both cyclopentadienyl and diphenylphosphinocyclopentadienyl ligands inclined to each other at 3.2 (1°). The $\text{Co}1\cdots\text{Cg}1$ and $\text{Co}1\cdots\text{Cg}2$ distances are 1.643 (2) and 1.637 (8) Å, respectively, and the $\text{Cg}1\cdots\text{Co}1\cdots\text{Cg}2$ angle is 175.9 (8°) ($\text{Cg}1$ and $\text{Cg}2$ are the centroids of the five-membered cyclopentadienyl and diphenylphosphinocyclopentadienyl rings, respectively).

Figure 1

The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Both disorder components are shown.

These rings are approximately eclipsed. The disordered PF_6^- anion links to the cobaltocenium cation *via* weak $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds (Fig. 2 and Table 2).

Experimental

The title compound was prepared according to the method of Brasse *et al.* (2000). Single crystals were obtained by slow diffusion of diethyl ether into a solution of the compound in acetone.

Crystal data

$[\text{Co}(\text{C}_5\text{H}_5)(\text{C}_{17}\text{H}_{14}\text{P})]\text{PF}_6$
 $M_r = 518.24$
 Monoclinic, $C2/c$
 $a = 36.813(3) \text{ \AA}$
 $b = 10.2263(8) \text{ \AA}$
 $c = 11.9059(9) \text{ \AA}$
 $\beta = 99.469(1)^\circ$
 $V = 4421.0(6) \text{ \AA}^3$
 $Z = 8$

$D_x = 1.557 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 4616 reflections
 $\theta = 2.2\text{--}26.0^\circ$
 $\mu = 0.98 \text{ mm}^{-1}$
 $T = 292(2) \text{ K}$
 Block, yellow
 $0.30 \times 0.30 \times 0.30 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.758, T_{\max} = 0.758$
 14389 measured reflections

4335 independent reflections
 3275 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.054$
 $\theta_{\text{max}} = 26.0^\circ$
 $h = -45 \rightarrow 39$
 $k = -12 \rightarrow 12$
 $l = -11 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.129$
 $S = 1.04$
 4335 reflections
 297 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.074P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$

Table 1

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

Co1—C1	2.008 (4)	C11—P1	1.836 (3)
C10—P1	1.826 (3)	C17—P1	1.829 (3)
C10—P1—C17	101.17 (12)	C17—P1—C11	103.59 (12)
C10—P1—C11	100.51 (11)		

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C8—H8 \cdots F2	0.98	2.45	3.133 (4)	127
C6—H6 \cdots F4 ⁱ	0.98	2.36	3.270 (5)	155
C4—H4 \cdots F3 ⁱⁱ	0.98	2.33	3.215 (5)	150
C1—H1 \cdots F5 ⁱ	0.98	2.51	3.167 (6)	124

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

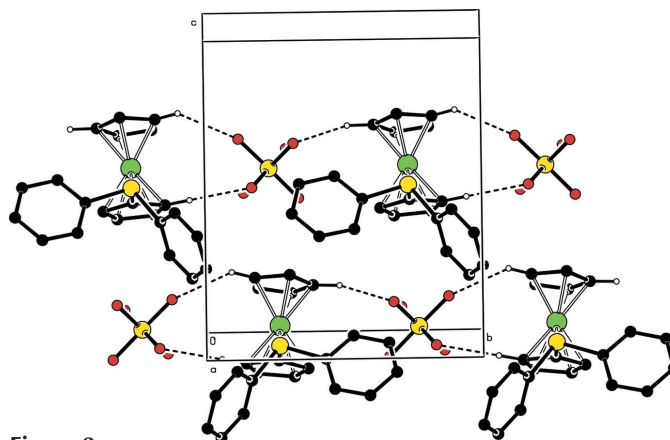


Figure 2

The packing of (I), showing the formation of chains along $[010]$. Hydrogen bonds are shown as dashed lines and, for the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. Only the major disorder component of the anion is shown.

At an early stage in the refinement, disorder was apparent in four of the F atoms of the hexafluorophosphate anion. The disordered F atoms were assigned the same isotropic displacement parameters, and bond distances in the minor disorder component were restrained. The non-H atoms in the minor component were refined isotropically. The occupation factors of the two components converged at 0.799 (6) and 0.201 (6). All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $\text{C}-\text{H} = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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

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