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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(C-C)$  = 0.009 Å  
 R factor = 0.060  
 wR factor = 0.184  
 Data-to-parameter ratio = 19.0

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

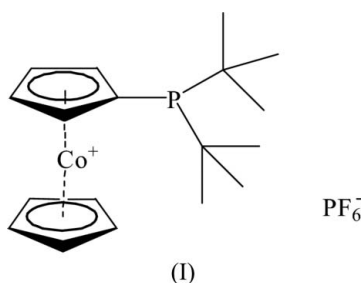
**(Di-*tert*-butylphosphino)cobaltocenium  
 hexafluorophosphate**

In the title compound,  $[Co(C_{18}H_{27}P)]PF_6$ , the P–C(cyclo-  
 pentadienyl) bond distance [1.840 (4) Å] is significantly  
 shorter than P–C(*tert*-butyl) bond distances [1.879 (5) and  
 1.900 (5) Å]. The  $PF_6^-$  anion links to the cobaltocenium  
 cation *via* weak C–H...F hydrogen bonding.

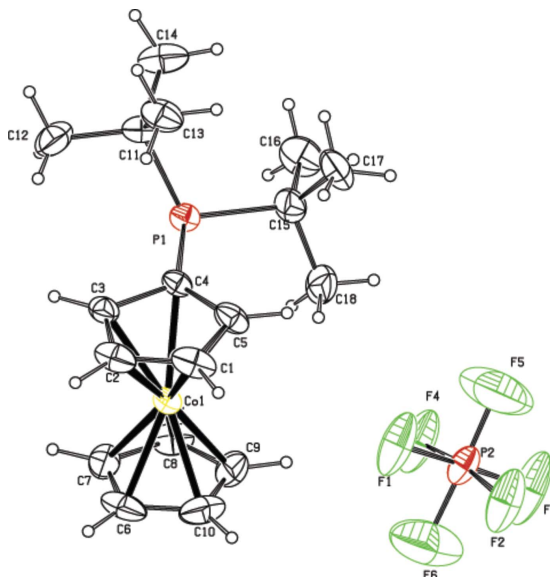
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**Comment**

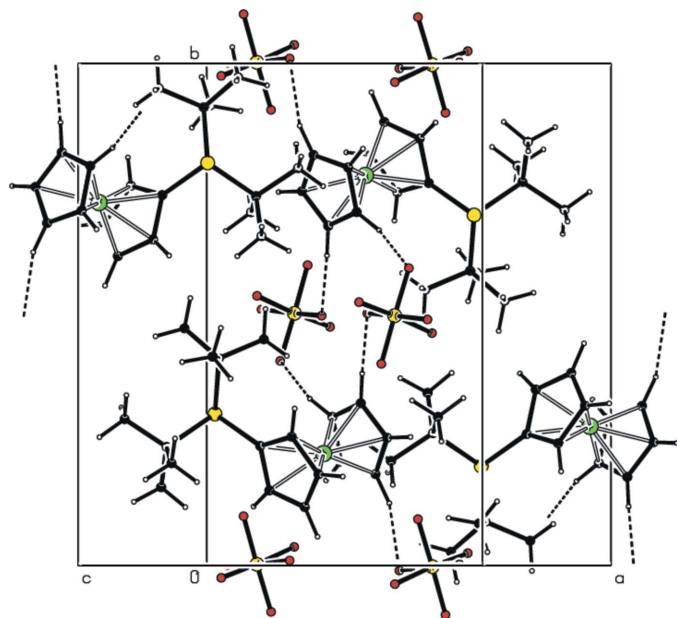
Cobaltocene derivatives have been applied in cross-coupling  
 areas (Christopher & Thomas, 2000). As part of an investiga-  
 tion on new catalysts, we have focused our attention on  
 cobaltocenium compounds. In this paper, we present the  
 crystal structure of the title compound, (I).



The molecular structure of (I) is shown in Fig. 1. The Co1–  
 C bond distances within the C1–C5 and C6–C10 rings range  
 from 2.005 (4) to 2.061 (4) Å and from 2.007 (5) to  
 2.026 (4) Å, respectively. The Co1...Cg1 and Co1...Cg2



**Figure 1**  
 The molecular structure of (I), with 30% probability displacement  
 ellipsoids (arbitrary spheres for H atoms).



**Figure 2**  
The packing of (I), showing the C—H...F hydrogen bonds as dashed lines.

distances are 1.639 (2) and 1.631 (2) Å, respectively, and the Cg1...Co1...Cg2 angle is 177.2 (7)°, where Cg1 and Cg2 are the centroids of the substituted and unsubstituted rings, respectively. The cyclopentadienyl C—C bond distances range from 1.395 (8) to 1.443 (5) Å (ring C1—C5) and from 1.364 (9) to 1.402 (7) Å (ring C6—C10). The P1—C4 bond distance is significantly shorter than the P1—C11 and P1—C15 distances (Table 1).

The PF<sub>6</sub><sup>−</sup> anion links to the cobaltocenium cation *via* the weak C—H...F hydrogen bonding (Fig. 2 and Table 2).

## Experimental

The title compound was prepared according to standard literature procedures (Claudia & Albrecht, 2000). Slow diffusion of diethyl ether into an acetone solution of the compound gave single crystals of (I).

### Crystal data

[Co(C <sub>18</sub> H <sub>27</sub> P)]PF <sub>6</sub>	$D_x = 1.456 \text{ Mg m}^{-3}$
$M_r = 478.27$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3154 reflections
$a = 12.2603$ (11) Å	$\theta = 2.2\text{--}22.1^\circ$
$b = 15.2255$ (12) Å	$\mu = 0.98 \text{ mm}^{-1}$
$c = 12.3230$ (11) Å	$T = 293$ (2) K
$\beta = 108.4620$ (11)°	Block, red
$V = 2181.9$ (3) Å <sup>3</sup>	$0.30 \times 0.30 \times 0.20 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD area-detector diffractometer	4754 independent reflections
$\varphi$ and $\omega$ scans	3415 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.030$
$T_{\text{min}} = 0.685$ , $T_{\text{max}} = 0.822$	$\theta_{\text{max}} = 27.0^\circ$
12636 measured reflections	$h = -9 \rightarrow 15$
	$k = -16 \rightarrow 19$
	$l = -15 \rightarrow 15$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.184$   
 $S = 1.03$   
 4754 reflections  
 250 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1021P)^2 + 0.9195P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.73 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

P1—C4	1.840 (4)	P1—C15	1.879 (5)
P1—C11	1.900 (5)		
C4—P1—C11	98.9 (2)	C11—P1—C15	111.6 (2)
C4—P1—C15	104.50 (19)		

**Table 2**

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
C6—H6...F2 <sup>i</sup>	0.98	2.49	3.340 (7)	145
C8—H8...F3 <sup>ii</sup>	0.98	2.45	3.349 (6)	152
C9—H9...F4	0.98	2.35	3.304 (8)	164

Symmetry codes: (i)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $-x + 1, -y + 1, -z + 1$ .

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles refined to fit the electron density, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . Other H atoms were placed in calculated positions, with C—H = 0.98 Å, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

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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