Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

[η^5-2-(Diphenylphosphino)-1-methylcyclopentadienyl](η^5-methylcyclopentadienyl)cobalt(III) hexafluorophosphate

Yan Chen, Guang-Ao Yu,* Xiang-Gao Meng and Sheng-Hua Liu

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

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

Received 31 December 2006
Accepted 18 January 2007

In the title cobaltocenium compound, [Co(C_6H_7)($C_{18}H_{16}$P)]-PF_6, the Co^{III} atom is bound to methylcyclopentadienenyl and η^5-2-(diphenylphosphino)-1-methylcyclopentadienyl ligands inclined to each other at 1.3 (2)°.

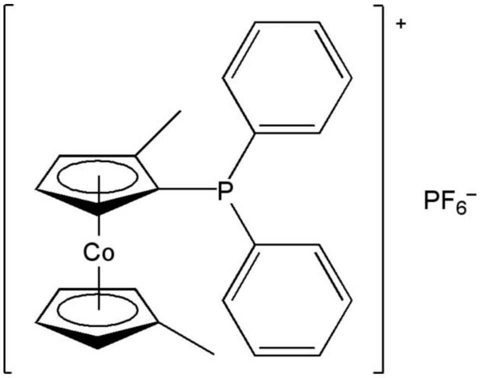
Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.053
wR factor = 0.144
Data-to-parameter ratio = 16.3

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

Comment

Cobaltocene derivatives have been applied as catalysts in hydroformylation reactions (Brasse *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). The crystal structure of a similar complex, [Co(C_5H_5)($C_{17}H_{14}$P)]PF_6 (Ren *et al.*, 2006), has been reported previously.



(I)

In (I) (Fig. 1), Co^{III} is bound to methylcyclopentadienenyl and (diphenylphosphino)methylcyclopentadienyl ligands, with the cyclopentadienyl rings approximately eclipsed and inclined to each other at 1.3 (2)°. The Co1$\cdots$*Cg*1 and Co1$\cdots$*Cg*2 distances are 1.6359 (17) and 1.6343 (15) Å, respectively, and the *Cg*1$\cdots$Co1$\cdots$*Cg*2 angle is 179.21 (9)° [*Cg*1 and *Cg*2 are the centroids of the C1–C5 and C7–C11 rings, respectively]. Atom C12 lies 0.030 (4) Å out of the mean plane of the C7–C11 ring. Atom C6 lies 0.016 (4) Å out of the mean plane of the C1–C5 ring, while P1 lies 0.069 (1) Å out of the same plane. One phenyl ring of the (diphenylphosphino)methylcyclopentadienyl ligand is disordered over two orientations.

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.

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Crystal data

$[Co(C_6H_7)(C_{18}H_{16}P)]PF_6$
$M_r = 546.29$
Monoclinic, $P2_1/n$
$a = 10.4454$ (6) Å
$b = 22.8701$ (13) Å
$c = 10.7218$ (6) Å
$\beta = 108.501$ (1)°
$V = 2428.9$ (2) Å^3
$Z = 4$
$D_x = 1.494$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.89$ mm^{-1}
$T = 297$ (2) K
Block, yellow
0.20 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: none
16458 measured reflections
5287 independent reflections
4078 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.038$
$\theta_{\rm max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.144$
$S = 1.05$
5287 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0763P)^2 + 0.6103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.49$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.24$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—C1	2.045 (3)	Co1—C7	2.062 (3)
Co1—C2	2.042 (3)	Co1—C8	2.023 (3)
Co1—C3	2.035 (3)	Co1—C9	2.007 (3)
Co1—C4	2.026 (3)	Co1—C10	2.015 (3)
Co1—C5	2.021 (3)	Co1—C11	2.030 (3)

At an early stage of the refinement, disorder was apparent in one phenyl ring of the 2-(diphenylphosphino)methylcyclopentadienyl ligand. Two components [C19–C24 and C19*A*—C24*A*] were modelled with geometries constrained to be regular hexagons. All C atoms were refined with anisotropic displacement parameters, and the site occupancy factors for the two components, constrained to sum to unity, were refined to 0.57 (3) and 0.43 (3). All H atoms were visible in difference Fourier maps, but were placed in geometrically idealized positions [C—H = 0.93 Å (CH) or 0.96 Å (CH_3)] and constrained to ride on their parent atoms with $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$, or $1.5U_{\rm eq}(C)$ for the methyl groups. The methyl groups were allowed to rotate about their local threefold axes.

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*.

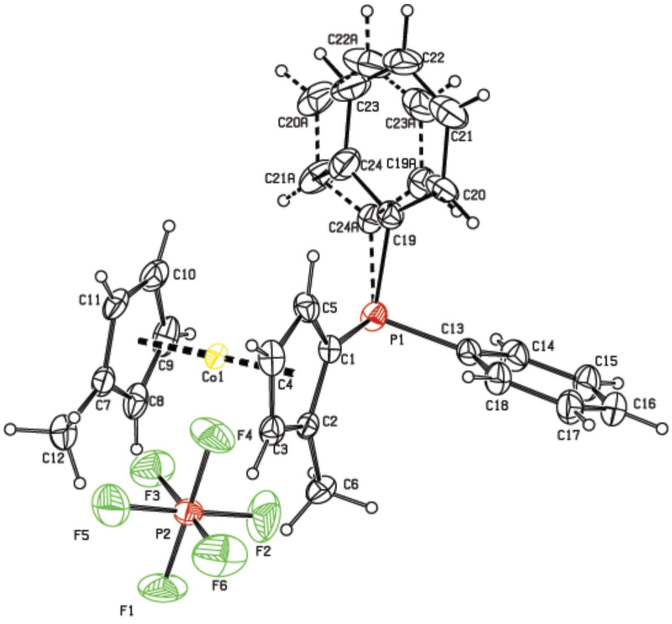

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. Both disorder components are shown.

We gratefully acknowledge financial support from the National Natural Science Foundation of China (No. 20572029), New Century Excellent Talents in University (NCET-04-0743), the Programme for Excellent Research Groups of Hubei Province (No. 2004ABC002), the Cultivation Fund of the Key Scientific and Technical Innovation Project, Ministry of Education of China (No. 705039), the National Key Project for Basic Research of China (No. 2004CCA00100), and the Natural Science Foundation of Hubei Province (No. 2005ABA038).

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