Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

(η^5-Cyclopentadienyl)[η^4-(*exo*-5-phenylethynyl)-1,3-cyclopentadienyl]cobalt(II)

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Received 10 October 2005
Accepted 3 January 2006

Key indicators

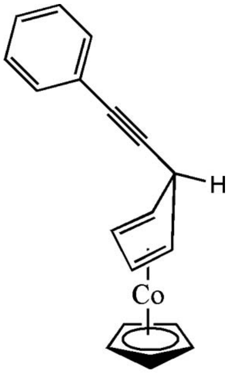
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.062
wR factor = 0.166
Data-to-parameter ratio = 11.7

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

In the crystal structure of the title compound, [Co(C_5H_5)($C_{13}H_{10}$)], the Co atom is connected to two five-membered rings. Both rings are disordered and were refined using a split model.

Comment

The cyclopentadienyl anion, C_5H_5 (Cp), is one of the most important ligands in the organometallic chemistry of transition metals (Jutzi *et al.*, 1994; Janiak *et al.*, 1991). Such ligands can stabilize metals in low and high oxidition states, while the easy change of hapticity (η^1, η^3 or η^5) of the Cp ligand allows it to be readily adaptable to changes in the electronic and steric requirements of the central atom (Philippopoulos *et al.*,1998). In this context, we have focused our attention on the preparation of cobaltocenium derivatives. The title compound, (I), is a synthetic intermediate from which different cobaltocenium derivatives with *e.g.* good solubility in polar solvents can be prepared.



(I)

In the structure of the title compound, both five-membered rings are disordered and were refined using a split model (Fig. 1). Atom C10 deviates significantly from the η^4(C_4H_4) ring plane; this is obvious from the torsion angles C10—C6—C7—C8, C7—C8—C9—C10 and C8—C9—C10—C6 (Table 1). Therefore, atoms C6, C7, C8, C9, C10 are not coplanar. The dihedral angle between the η^4(C_4H_4) ring plane and the plane formed by C6, C9 and C10 is 29.4 (1)°.

Experimental

The title compound was synthesized according to literature procedures (Wildschek *et al.*,1990). Crystals appropriate for data collection were obtained by slow evaporation of a mixed dichloromethane and hexane solution (2:1 *v*/*v*) at room temperature.

Crystal data

$[\mathrm{Co(C_5H_5)(C_{13}H_{10})}]$
$M_r = 290.23$
Monoclinic, $P2_1/c$
$a = 6.0403$ (7) Å
$b = 17.926$ (2) Å
$c = 12.9002$ (14) Å
$\beta = 92.134$ (2)°
$V = 1395.9$ (3) Å^3
$Z = 4$
$D_x = 1.381$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 879 reflections
$\theta = 2.3$–16.9°
$\mu = 1.21$ mm^{-1}
$T = 292$ (2) K
Needle, red
0.40 × 0.10 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6946 measured reflections
2443 independent reflections
1450 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.056$
$\theta_{\max} = 25.0°$
$h = -7 \rightarrow 7$
$k = -21 \rightarrow 18$
$l = -13 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.166$
$S = 1.04$
2443 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.4218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.45$ e Å^{-3}
$\Delta\rho_{\min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C10—C11	1.499 (7)	C12—C13	1.435 (7)
C11—C12	1.178 (7)		
C7—C6—C10	112.2 (8)	C9—C10—C6	89.3 (6)
C8—C9—C10	116.9 (8)		
C10—C6—C7—C8	−21.6 (10)	C7—C8—C9—C10	23.6 (9)
C6—C7—C8—C9	−0.6 (9)	C8—C9—C10—C6	−32.7 (8)

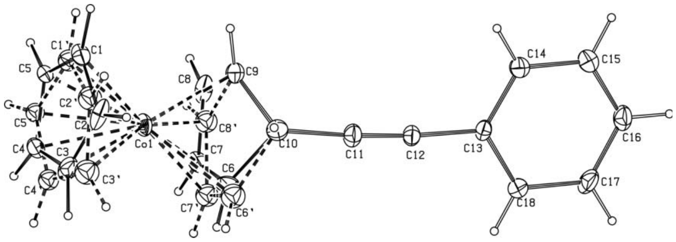


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probablity level. Both disorder components of each ring are shown.

It was apparent at an early stage of the refinement that both five-membered rings were disordered. They were therefore refined using a split model with DFIX restraints (*SHELXS97*; Sheldrick, 1997) of C═C = 1.40 (1) Å, C—C = 1.52 (1) Å for the C—C distances. The major component was refined anisotropically whereas the minor component was refined isotropically. However, for some atoms the disorder could not be resolved and therefore they show enlarged anisotropic displacement parameters. The site-occupation factors for the disordered atoms were refined to 0.58 (4) and 0.42 (4), respectively, for the major and minor components of the cyclopentadienyl ring, and to 0.64 (3) and 0.36 (3), respectively, for the major and minor components of atoms C6–C8. H atoms were positioned geometrically, with C—H distances in the range 0.93–0.98 Å, and refined as riding, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); 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*.

The authors acknowledge financial support from the National Natural Science Foundation of China (No. 20472023), New Century Excellent Talents in Universities (NCET-04-0743), the Hubei Province Science Fund for Distinguished Young Scholars (No. 2003ABB006) and the Natural Science Foundation of Hubei Province (No. 2005ABA038).

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Acta Cryst. (2006). E**62**, m262–m263 Li *et al.* • $[\mathrm{Co(C_5H_5)(C_{13}H_{10})}]$ **m263**