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Dichloro(η^5-pentamethylcyclopentadienyl)-(pyridine-*N*)rhodium

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Key indicators

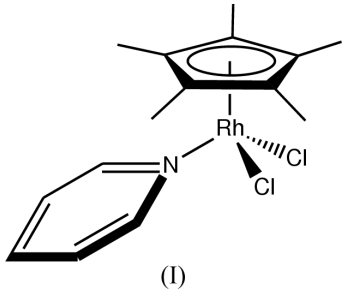
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.016
wR factor = 0.046
Data-to-parameter ratio = 17.0

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

In the title compound, $[RhCl_2(C_{10}H_{15})(C_5H_5N)]$, the Rh atom displays a piano-stool configuration. The two halves of the molecule are related by mirror symmetry.

Comment

The structure of the title compound, (I) (Fig. 1), is comparable to the previously reported ruthenium analog, dichloro(η^5-pentamethylcyclopentadienyl)(pyridine-*N*)ruthenium (Bottomley & Sutton, 1992). The Rh atom displays a piano-stool configuration. The two halves of the molecule are related by symmetry. The Rh, N, C1, C8 and C11 atoms, as well as H8 and H11*B*, lie on a mirror plane. The Rh—*Cp** distance (*Cp** is the centroid of the cyclopentadienyl ring) of 1.771 (1) Å is slightly longer than that reported for $[(\eta^5\text{-}C_5Me_5)_2Rh_2(\mu\text{-}Cl)_2Cl_2]$ (1.7558 Å; Churchill *et al.*, 1977).



(I)

Experimental

The title compound was synthesized by a previously described procedure (Kang *et al.*, 1969). Crystals were obtained by slow evaporation of a benzene solution.

Crystal data

$[RhCl_2(C_{10}H_{15})(C_5H_5N)]$
M_r = 388.13
Monoclinic, $P2_1/m$
a = 7.1501 (14) Å
b = 13.185 (3) Å
c = 8.4979 (17) Å
β = 106.45 (3)°
V = 768.4 (3) Å^3
Z = 2
D_x = 1.678 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4203 reflections
θ = 2.5–26.4°
μ = 1.45 mm^{-1}
T = 150 (2) K
Prism, red
0.38 × 0.06 × 0.05 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.610, T_{max} = 0.931
4626 measured reflections
1631 independent reflections
1549 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 26.4°
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 16$
$l = -10 \rightarrow 10$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.046$
$S = 1.11$
1631 reflections
96 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0240P)^2 + 0.3726P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.024$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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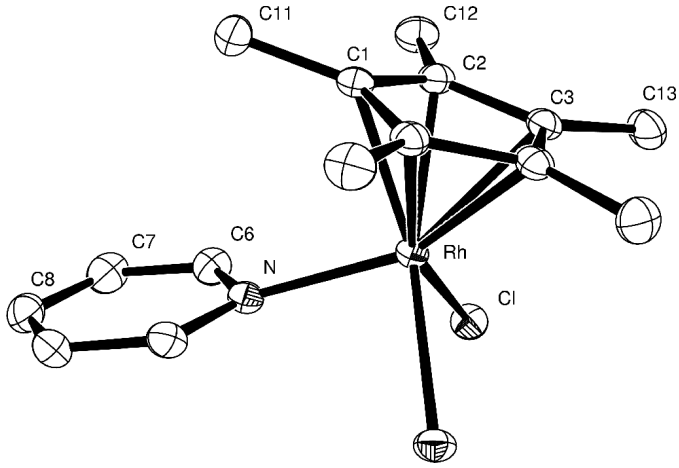

Figure 1
ORTEP view of (I) showing displacement ellipsoids at the 50% probability level.

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