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Carbonyliodo{[1-(2-pyridylmethyl)cyclohexylmethyl]-η^5-cyclopentadienyl-κN}ruthenium(II)

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Key indicators

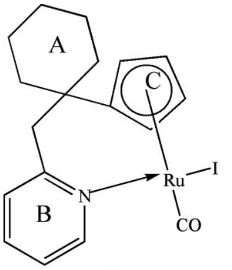
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.008 Å
R factor = 0.036
wR factor = 0.119
Data-to-parameter ratio = 20.1

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

In the title compound, $[Ru(C_{17}H_{20}N)I(CO)]$, the distance between the Ru atom and the centroid of the cyclopentadiene ring is 1.850 (2)Å. The dihedral angle between the planes of the pyridine and cyclopentadiene rings is 53.8 (2)°.

Comment

The chemistry of cyclopentadiene metal complexes containing a donor-functionalized side chain has been receiving extensive attention (Jutzi & Redeker, 1998; Jutzi & Siemeling, 1995). For the pyridyl side-chain-functionalized cyclopentadiene ligands, the N atom can act as a good two-electron donor site and can coordinate to Ru, such as in the title compund, (I).



(I)

In (I) (Fig. 1), the Rh—Cp* distance (Cp* is the centroid of the cyclopentadiene ring) is 1.850 (2) Å. The Cp*—Ru1—I1, Cp*—Ru1—N1 and Cp*—Ru1—C18 angles are 123.75 (10), 122.80 (12) and 128.29 (17)°, respectively. The dihedral angle between the planes of the pyridine and cyclopentadiene rings is 53.8 (2)°. The cyclohexane ring adopts a chair conformation. In the crystal structure, inversion-related molecules form a C—H···O hydrogen-bonded dimer (Table 2).

Experimental

Bis({[1-(pyridin-2-ylmethyl)cyclohexyl]methyl}cyclopentadienyl)-tetra(carbonyl) diruthenium, (II) (0.705 mmol), was prepared from 2-[1-(cyclopenta-2,4-dienyl)cyclohexyl]pyridine (1.41 mmol) and dodecacarbonyltriruthenium (0.46 mmol) under refluxing xylene for 12 h (Chen *et al.*, 2006). Compound (I) was prepared from compound (II) (0.705 mmol) and iodine (0.705 mmol). Red single crystals suitable for X-ray diffraction were obtained by slow evaporation of a dichloromethane–hexane solution (1:1) at room temperature.

Crystal data

$[Ru(C_{17}H_{20}N)I(CO)]$
$M_r = 494.32$
Monoclinic, $P2_1/c$
$a = 6.7349\ (13)$ Å
$b = 22.903\ (5)$ Å
$c = 11.626\ (2)$ Å
$\beta = 99.29\ (3)°$
$V = 1769.8\ (6)$ Å^3

$Z = 4$
$D_x = 1.855$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.63$ mm^{-1}
$T = 296\ (2)$ K
Block, red
0.36 × 0.32 × 0.30 mm

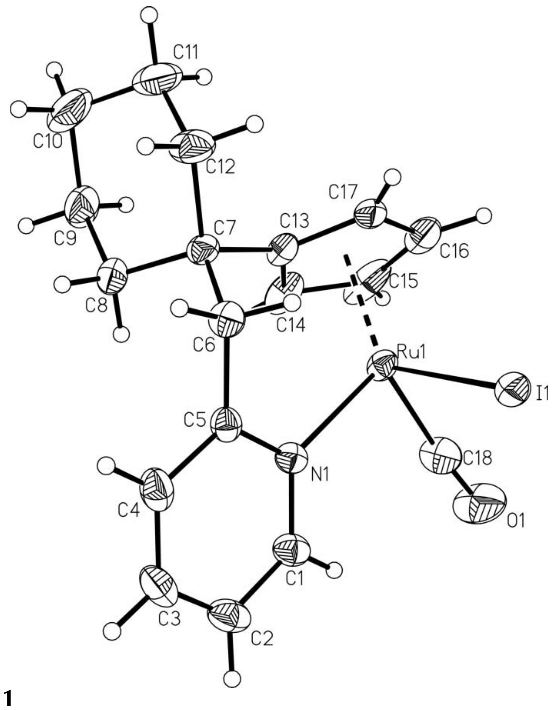


Figure 1

A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.451$, $T_{\max} = 0.506$ (expected range = 0.405–0.454)
17030 measured reflections
4026 independent reflections
3435 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.057$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.119$
$S = 1.13$
4026 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.063P)^2 + 0.677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.95$ e Å^{-3}
$\Delta\rho_{\min} = -1.37$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0093 (8)

Table 1

Selected geometric parameters (Å, °).

N1—Ru1	2.139 (3)	Ru1—C16	2.200 (5)
Ru1—C18	1.872 (5)	Ru1—C17	2.242 (5)
Ru1—C14	2.173 (5)	Ru1—C13	2.245 (4)
Ru1—C15	2.178 (5)	Ru1—I1	2.7016 (8)
C18—Ru1—N1	95.00 (18)	N1—Ru1—I1	87.17 (9)
C18—Ru1—I1	88.43 (19)		

Table 2

Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C15—H15⋯O1$^{\rm i}$	0.98	2.53	3.405 (9)	148

Symmetry code: (i) $-x, -y+1, -z+1$.

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.98 Å and $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C). In the absence of significant anomalous scattering effects, Friedel pairs were averaged. The deepest hole in the difference map is located at (1.0283, 0.1801, 0.4920).

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXL97*.

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