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Dicarbonyl(η^5-cyclopentadienyl)iodoruthenium(II)

Muhammad D. Bala,* Apollinaire Munyaneza and Neil J. Coville

Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg 2050, South Africa

Correspondence e-mail: mdbala@chem.wits.ac.za

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(O–C) = 0.008 Å
Disorder in main residue
R factor = 0.031
wR factor = 0.101
Data-to-parameter ratio = 16.7

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

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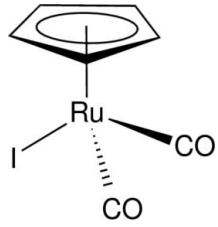
The title compound, $[Ru(C_5H_5)I(CO)_2]$, has a three-legged piano-stool geometry with a distorted pseudo-octahedral structure. The cyclopentadienyl ring is disordered over two sets of positions.

Comment

The title compound, (I), is a widely used and easily prepared precursor for a variety of organometallic ruthenium complexes. While some similar complexes with substituted Cp rings (Duraczyn'ska & Nelson, 2003; Barthel-Rosa *et al.*, 1997; Bhaduri *et al.*, 1994) and the corresponding iron complex, η^5-$CpFe(CO)_2I$ (Zeller *et al.*, 2003), have been reported, this compound with a simple Cp ring has not yet been structurally characterized.



(I)

The compound has a three-legged piano-stool geometry, with a distorted pseudo-octahedral structure around Ru. The cyclopentadienyl ring is disordered over two sets of positions, with site occupancies of 0.74 (2) and 0.26 (2) for the major and minor positions, respectively. All bond lengths and angles are in agreement with values reported for similar complexes.

Experimental

A solution of ruthenium carbonyl, $[Ru_3(CO)_{12}]$ (0.4 g) in dicyclopentadiene–heptane (2:3, 10 ml) was refluxed overnight, yielding the reddish crystalline dimer $[\eta^5\text{-}Cp(CO)_2Ru]_2$ quantitatively. The title complex, η^5-$CpRu(CO)_2I$, (I), was readily obtained by reacting the dimer (0.3 g) with iodine (0.2 g) in tetrahydrofuran (10 ml) for 1 h at room temperature.

Crystal data

$[Ru(C_5H_5)I(CO)_2]$
M_r = 349.08
Monoclinic, $P2_1/c$
a = 6.7702 (2) Å
b = 10.0609 (3) Å
c = 13.4272 (4) Å
β = 102.257 (2)°
V = 893.74 (5) Å^3
Z = 4
D_x = 2.594 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 5.16 mm^{-1}
T = 173 (2) K
Plate, orange
0.31 × 0.26 × 0.11 mm

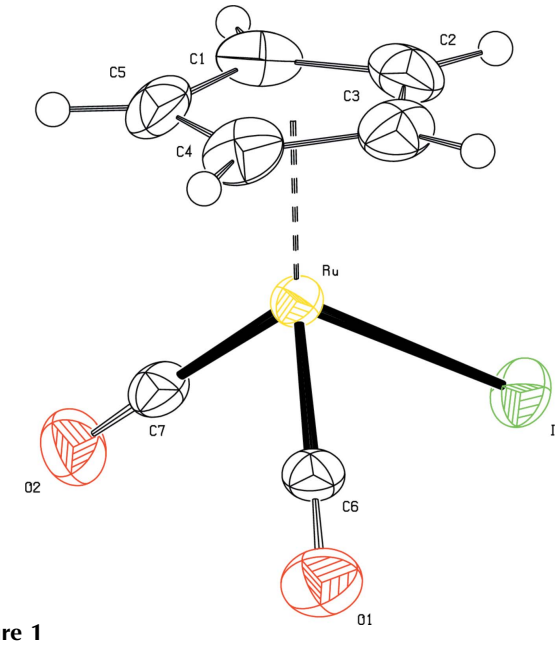


Figure 1
A view of the title complex. Displacement ellipsoids are drawn at the 50% probability level. Only one component of the disordered Cp ring is shown.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.220, T_{max} = 0.571
6750 measured reflections
2139 independent reflections
1898 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 28.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.101
S = 1.23
2139 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 5.0769P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.37 e Å^{-3}
$\Delta\rho_{min}$ = −1.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

*Cg*1 and *Cg*2 are the centroids of the major and minor components of ring C1–C5.

C6—O1	1.158 (7)	I—Ru	2.7009 (6)
C6—Ru	1.869 (6)	*Cg*1—Ru	1.888 (4)
C7—O2	1.172 (7)	*Cg*2—Ru	1.874 (12)
C7—Ru	1.865 (6)		
C7—Ru—O2	178.7 (5)	C6—Ru—O1	179.1 (5)

The H atoms were positioned geometrically and allowed to ride on their parent atoms during refinement, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The disordered Cp ring was refined with similarity restraints (SIMU and DELU) for the geometry of the two components.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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