Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

(*n*-Butyldiphenylphosphine)dichloro(η^6-*p*-cymeme)ruthenium(II)

Giuseppe Bruno *et al.*

Electronic paper
This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

(*n*-Butyldiphenylphosphine)dichloro-(η^6-*p*-cymeme)ruthenium(II)

Giuseppe Bruno,* Manuela Panzalorto, Francesco Nicoló, Carmela Grazia Arena and Paola Cardiano

Dip. di Chimica Inorganica, Chimica Analitica e Chimica Fisica, Universitá di Messina, 98166 Vill. Sant'Agata, Messina, Italy
Correspondence e-mail: bruno@medif0.unime.it

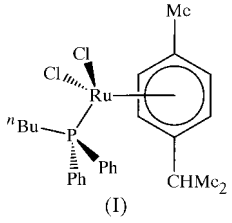
Received 20 July 2000
Accepted 25 August 2000

Data validation number: IUC0000230

The title ruthenium complex, $[RuCl_2(C_{10}H_{14})(C_{16}H_{19}P)]$, contains a monodentate $(C_4H_9)PPh_2$ ligand coordinated by the P atom. Coordination about the metal centre is completed by a η^6-*p*-cymene ligand and two Cl atoms.

Comment

The η^6-arene complexes of Ru^{II} have shown promising results in the catalytic hydrogenation of olefins. Furthermore, complexes of this type have been successfully employed in asymmetric olefin hydrogenation. The structure of (*n*-butyldiphenylphosphine)dichloro(η^6-*p*-cymeme)ruthenium(II), (I), is presented here.



(I)

Experimental

The title compound was synthesized by reaction of $[RuCl_2(p\text{-cymene})]$ and $^n BuPh_2P$ in tetrahydrofuran in a 1:2 molar ratio and crystals were obtained by slow evaporation of a CH_2Cl_2/hexane solution.

Crystal data

$[RuCl_2(C_{10}H_{14})(C_{16}H_{19}P)]$	D_x = 1.421 Mg m^{-3}
M_r = 548.46	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 30 reflections
a = 10.574 (3) Å	θ = 13–30°
b = 12.983 (4) Å	μ = 0.894 mm^{-1}
c = 19.239 (6) Å	T = 293 (2) K
β = 103.99 (2)°	Regular prismatic, red
V = 2562.8 (13) Å^3	0.50 × 0.20 × 0.14 mm
Z = 4	

Data collection

Siemens *R*3*m*/*V* diffractometer	$h = -2 \rightarrow 12$
ω–2θ scans	$k = 0 \rightarrow 15$
4878 measured reflections	$l = -22 \rightarrow 22$
4530 independent reflections	3 standard reflections every 197 reflections
2393 reflections with $I > 2\sigma(I)$	intensity decay: 2.3%
R_{int} = 0.0170	
θ_{max} = 25.04°	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.057	$w = 1/[\sigma^2(F_o^2) + (0.0880P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.159	$(\Delta/\sigma)_{max} < 0.001$
S = 0.864	$\Delta\rho_{max}$ = 1.378 e Å^{-3}
4530 reflections	$\Delta\rho_{min}$ = −0.868 e Å^{-3}
265 parameters	

Table 1
Selected geometric parameters (Å, °).

Ru—C5	2.170 (8)	Ru—C2	2.241 (8)
Ru—C4	2.176 (8)	Ru—P	2.352 (2)
Ru—C1	2.225 (8)	Ru—Cl1	2.413 (2)
Ru—C6	2.225 (8)	Ru—Cl2	2.413 (2)
Ru—C3	2.228 (8)		
P—Ru—Cl1	87.06 (8)	Cl1—Ru—Cl2	88.47 (8)
P—Ru—Cl2	83.51 (7)		

The H atoms were located on idealized positions and allowed to ride on the their parent C atoms (U_{iso} = 0.08 Å^2).

Data collection: *P*3/V (Siemens, 1989); cell refinement: *P*3/*V*; data reduction: *XDISK* (Siemens, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: locally modified *PARST*95 (Nardelli, 1995) and *SHELXL*97.

We would like to express our gratitude, for support and aid, to the Italian MURST and to the 'Centro Interdipartimentale di Servizi per la Diffrattometria a Raggi X' of the University of Messina.

References

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Siemens (1989). *P*3/*V*. Release 4.21/V. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1990). *XDISK*. Release 4.21/V. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.