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Dichloro[3-(1-naphthylmethyl)-1-(2,4,6-trimethylbenzyl)imidazolidin-2-ylidene]ruthenium

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.063
Data-to-parameter ratio = 14.3

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

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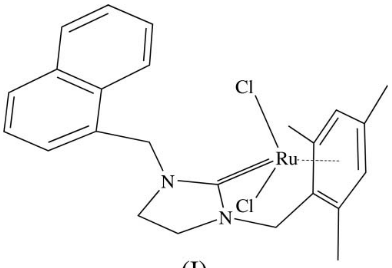
In the title compound, [$RuCl_2(C_{24}H_{26}N_2)$], the multidentate ligand functions as both an arene and a carbene, and occupies four coordination sites. The two Cl atoms complete a distorted octahedron about the Ru atom.

Comment

N-Heterocyclic carbenes have recently emerged as an important family of ligands with electronic characteristics similar to those of phosphines (Bourissou *et al.*, 2000). Complexes containing imidazolin-2-ylidenes, which are neutral two-electron-donor ligands with negligible π-back-bonding characteristics, are also thermally stable. This latter feature represents an essential prerequisite for the synthesis of highly efficient catalysts. Recently, we described a novel series of imidazolidine derivatives and their ruthenium complexes (Çetinkaya, Özdemir, Bruneau & Dixneuf, 1997; Çetinkaya, Özdemir & Dixneuf, 1997; Çetinkaya *et al.*, 2002; Özdemir *et al.* 2001; Arslan, Vanderveer, Özdemir, Çetinkaya & Demir, 2004, 2005; Arslan, Vanderveer, Özdemir, Çetinkaya & Yaşar, 2004). One of these new derivatives is the title compound, (I), the structure of which is described here.



(I)

The ligand in (I) has both an imidazolidine and an arene ring, which is connected to the former *via* a CH_2 bridge (see Fig. 1). This configuration leads to a system with very little apparent strain when coordinating the Ru atom. The complex is best thought of as containing an octahedrally coordinated Ru center with the arene residue occupying three sites, the remaining sites being occupied by an Ru=C bond, derived from the imidazole ring, and two Ru—Cl bonds. The complex has a similar arrangement to both dichloro[*N*-(2,4,6-trimethylbenzyl)-*N*-(2-methoxyethyl)imidazolidin-2-ylidene]ruthenium and dichloro[*N*-(2,4,6-trimethylbenzyl)-*N*-(*n*-butyl)imidazolidin-2-ylidene]ruthenium, as described recently (Arslan *et al.* 2005).

The small steric demand of the imidazolidine ligand is reflected in the C(11)—Ru—C1(1),Cl(2) angles of 101.33 (8) and 83.70 (8)°, respectively, a result that reflects the situation

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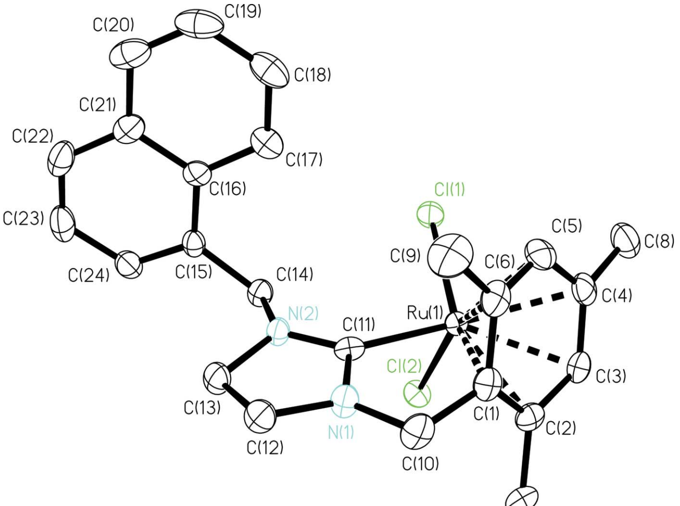

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

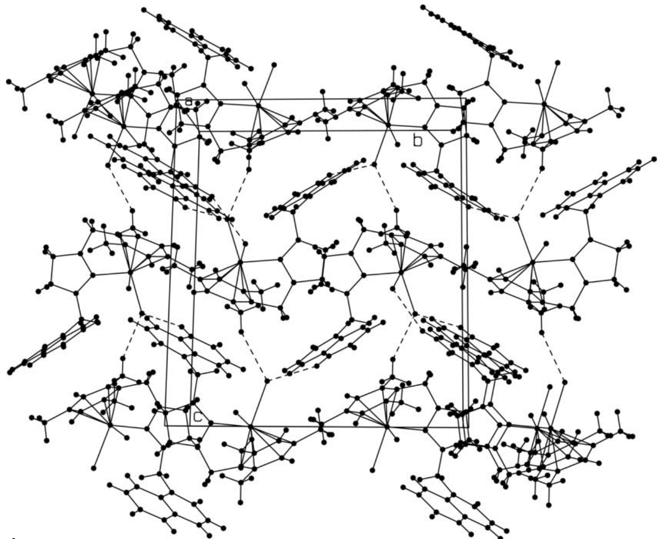

Figure 2
Packing diagram for (I) viewed along [100]. Dashed lines indicate hydrogen bonds.

found in related Ru complexes (Çetinkaya *et al.*, 2003; Arslan *et al.*, 2005). The Ru—Cl bond lengths differ somewhat (see Table 1). The Ru—carbene distance, Ru(1)—C(11), of 2.035 (3) Å, matches the literature data (Çetinkaya *et al.*, 2003; Arslan *et al.*, 2005). The atoms comprising the 2,4,6-trimethylbenzyl ring are coplanar, the mean deviation from their least-squares plane being 0.031 (2) Å.

The crystal packing shows the molecule stacked in a parallel sheet along [100] (Fig. 2). Intramolecular interactions are C(20)—H(20)···Cl(1), with H···Cl = 2.89 Å and an angle at H of 159°, C(7)—H(7*A*)···Cl(1), with H···Cl = 2.90 Å and an angle of 150°, and C(23)—H(23)···Cl(2), with H···Cl = 2.86 Å and an angle of 150°.

Experimental

A solution of tetraaminoethene (1.1 mmol) and $[RuCl_2(\eta^6\text{-}C_6Me_6)]_2$ (1.0 mmol) in toluene (10 ml) was heated in an oil bath (383 K) for 4 h. After cooling to 298 K, hexane (10 ml) was added and the solution was cooled to 258 K. The precipitated orange solid was filtered off and recrystallized from dichloromethane–diethyl ether (10:30 ml); the complex was isolated in 75% yield. M.p. 600–601 K. Analysis calculated for $C_{24}H_{26}Cl_2N_2Ru$: C 56.03, H 5.09, N 5.45%; found: C 57.15, H 5.01, N 5.52%. ^{1}H NMR ($CDCl_3$): δ 2.19 (*s*, 3H, Me—C8), 2.27 (*s*, 6H, Me—C6, 9), 3.14 (*t*, 2H, *J* = 7.6 Hz, CH_2—C12), 3.70 (*t*, 2H, *J* = 8.0 Hz, CH_2—C13), 4.58 (*s*, 2H, CH_2—C10), 5.12 (*s*, 2H, CH_2—C14), 6.85 (*s*, 2H, CH—C3, C5), 7.39–8.26 (*m*, 7H, CH—C17—C20; C22—C24).

Crystal data

$C_{24}H_{26}Cl_2N_2Ru$
$M_r = 514.44$
Monoclinic, $P2_1/c$
$a = 8.6515$ (10) Å
$b = 14.721$ (2) Å
$c = 16.734$ (3) Å
$\beta = 97.702$ (4)°
$V = 2112.0$ (5) Å^3
$Z = 4$

$D_x = 1.618$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12915 reflections
$\theta = 2.5$–25.7°
$\mu = 1.01$ mm^{-1}
$T = 173$ (2) K
Prism, orange
0.24 × 0.17 × 0.14 mm

Data collection

Rigaku AFC-8*S* diffractometer
ω scans
Absorption correction: multi-scan (*REQAB*; Rigaku/MSC, 1999)
$T_{min} = 0.794$, $T_{max} = 0.872$
17997 measured reflections
3799 independent reflections

3364 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.2$°
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 17$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.063$
$S = 1.06$
3799 reflections
265 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2 + 2.5856P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru(1)—C(1)	2.108 (3)	Ru(1)—Cl(2)	2.4106 (7)
Ru(1)—C(2)	2.155 (3)	N(1)—C(10)	1.454 (4)
Ru(1)—C(3)	2.277 (3)	N(1)—C(11)	1.357 (3)
Ru(1)—C(4)	2.312 (3)	N(1)—C(12)	1.468 (4)
Ru(1)—C(5)	2.182 (3)	N(2)—C(11)	1.339 (4)
Ru(1)—C(6)	2.194 (3)	N(2)—C(13)	1.476 (4)
Ru(1)—C(11)	2.035 (3)	N(2)—C(14)	1.456 (4)
Ru(1)—Cl(1)	2.4412 (8)		
C(11)—Ru(1)—C(1)	78.79 (11)	C(11)—Ru(1)—Cl(1)	101.33 (8)
C(11)—Ru(1)—C(2)	103.99 (11)	C(11)—Ru(1)—Cl(2)	83.70 (8)
C(11)—Ru(1)—C(3)	141.84 (10)	Cl(2)—Ru(1)—Cl(1)	88.77 (3)
C(11)—Ru(1)—C(4)	154.98 (11)	Ru(1)—C(11)—N(1)	115.4 (2)
C(11)—Ru(1)—C(5)	120.34 (11)	Ru(1)—C(11)—N(2)	137.0 (2)
C(11)—Ru(1)—C(6)	87.69 (11)		

H atom positions were positioned on the basis of ideal geometries and were allowed to ride on their respective C atoms during refinement. All C—H distances were fixed at 0.96 Å, with $U_{iso}(H) = 1.5U_{eq}$(methyl C) and $U_{iso}(H) = 1.2U_{eq}(C)$ for the remaining atoms.

Data collection: *CrystalClear* (Rigaku/MSC, 1999); cell refinement: *CrystalClear*; data reduction: *SHELXTL* (Sheldrick, 1998); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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