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(η^6-Benzene)chlorido[2-(pyridin-2-yl)quinoline-κ^2N,N']ruthenium(II) tetrafluoridoborate

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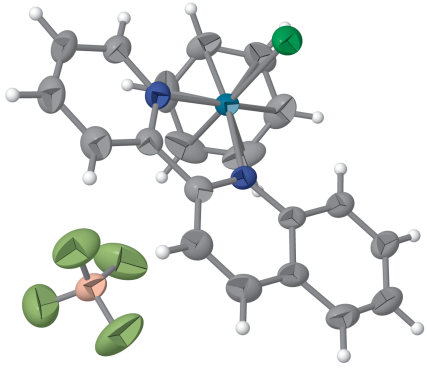
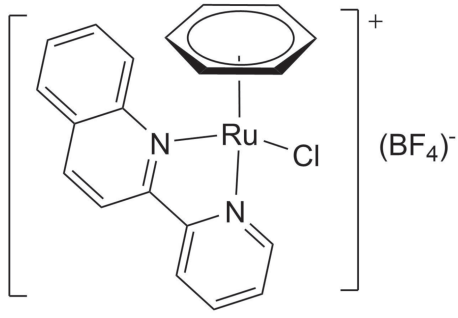
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[RuCl(C_6H_6)(C_{14}H_{10}N_2)]BF_4$ or $[Ru(\eta^6\text{-benzene})(L)Cl]^+BF_4^-$ [where L denotes the 2-(pyridin-2-yl)quinoline ligand], crystallizes in the monoclinic space group $P2_1/c$. The coordination environment around Ru^{II} is best described as pseudo-octahedral, resembling the familiar half-sandwich 'three-legged piano-stool' shape. In the coordination sphere, the η^6-binding benzene ligand coordinates with the central Ru^{II} atom occupying the 'seat' of the stool with a metal-to-centroid distance of 1.695 (17) Å, while the chelate ligand L coordinates with its N atoms and, together with the Cl ligand, defines the 'legs' of the stool. Apart from Coulombic forces, C—H···F and C—H···Cl hydrogen-bonding interactions consolidate the crystal packing.

3D view



Chemical scheme



Structure description

Ruthenium complexes exhibit a plethora of applications in the domains of medicinal chemistry (Casini & Pöthig, 2024; Rajendiran *et al.*, 2012; Chan *et al.*, 2017; Puckett & Barton, 2007), catalysis (Chavarot *et al.*, 2003; Ngo & Do, 2020; Hamelin *et al.*, 2007), and materials chemistry (Ryabov *et al.*, 2005; Huisman *et al.*, 2016; Vatsa & Padhi, 2021). Understanding their structural properties provides new insight into the design of novel ruthenium(II) complexes and predict their structure–activity relationships. In this context, the mononuclear mixed-ligand ruthenium(II) complex, $[Ru(\eta^6\text{-benzene})(L)Cl]^+BF_4^-$ [where L is 2-(pyridin-2-yl)quinolone] has been synthesized and characterized by single-crystal X-ray analysis in the present work.

The distinctive half-sandwich, 'three-legged piano-stool' geometry of the complex cation of the title compound (Fig. 1) is characteristic of numerous η^6-binding arene–ruthenium(II) complexes (Khamrang *et al.*, 2016; Zamisa *et al.*, 2024). The 'legs' of the

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···F4^{i}	0.93	2.48	3.375 (5)	162
C16—H16···F1	0.93	2.24	3.148 (6)	162
C19—H19···Cl1^{ii}	0.93	2.65	3.429 (4)	142

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

stool are defined by two σ-bonding N atoms from the chelating ligand *L* and the chlorido ligand, while the 'seat' is defined by the π-bonded benzene. The Ru^{II}-to-benzene(centroid) distance is 1.695 (17) Å and is comparable with other complexes containing *N*,*N*′-chelating ligands (Kelani *et al.*, 2023, 2024; Tsolis *et al.*, 2018). The Ru1—$N1_{py}$ bond [2.086 (3) Å] is slightly shorter than the Ru1—$N2_{qn}$ bond [2.147 (3) Å], revealing the pyridyl (py) N atom more firmly coordinates the central Ru^{II} atom than the quinolone (qn) N atom. The bidentate ligand has a bite angle of N1—Ru1—N2 = 76.42 (10)°. A similar type of coordination is observed in the crystal structure of [((2,2′-bipyridyl)(η^6-*p*-cymene)iodido)-ruthenium(II)] hexafluoridophosphate (Kelani *et al.*, 2023). The chlorido ligand bonds to the Ru^{II} atom with a distance of 2.3840 (9) Å. Except for the Ru—Cl bond, all other bonds are slightly longer than in the structure of the related complex $[Ru(\eta^6\text{-}p\text{-cymene})LCl]^+(PF_6)^-$ (Tsolis *et al.*, 2018).

In the crystal, intermolecular C—H···F and C—H···Cl hydrogen bonding (Table 1) plays a crucial role in the crystal packing (Fig. 2).

Synthesis and crystallization

$[Ru(\eta^6\text{-benzene})Cl]_2$ (0.12 g, 0.2 mmol) and *L* (2-(pyridin-2-yl)quinolone) (0.1 g, 0.4 mmol) were suspended in methanol (20 ml) and stirred at room temperature for 2 h. A solution of $NaBF_4$ (200 mg, 0.60 mmol) in methanol (10 ml) was added to the initially orange solution, which changed color to yellow. After 24 h, the solution was evaporated, and the solid obtained was filtered off. The residue was washed with diethyl ether (40 ml) and dried under vacuum. The obtained product was recrystallized from a DCM:hexane mixture to give orange crystals. Yield: 65%.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[RuCl(C_6H_6)(C_{14}H_{10}N_2)]BF_4$
M_r	507.68
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	8.4191 (3), 23.1476 (9), 9.9079 (3)
β (°)	94.709 (3)
V (Å^3)	1924.35 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.00
Crystal size (mm)	0.65 × 0.50 × 0.41
Data collection	
Diffractometer	Agilent Xcalibur, Atlas, Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.507, 0.578
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8112, 4311, 3815
R_{int}	0.018
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.675
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.093, 1.13
No. of reflections	4311
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.92, −0.66

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

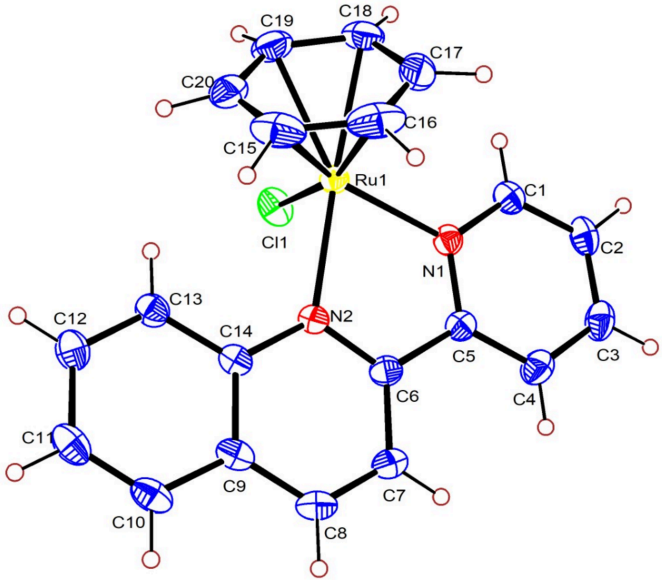


Figure 1
The molecular structure of the complex cation of the title compound with displacement ellipsoids at the 50% probability level.

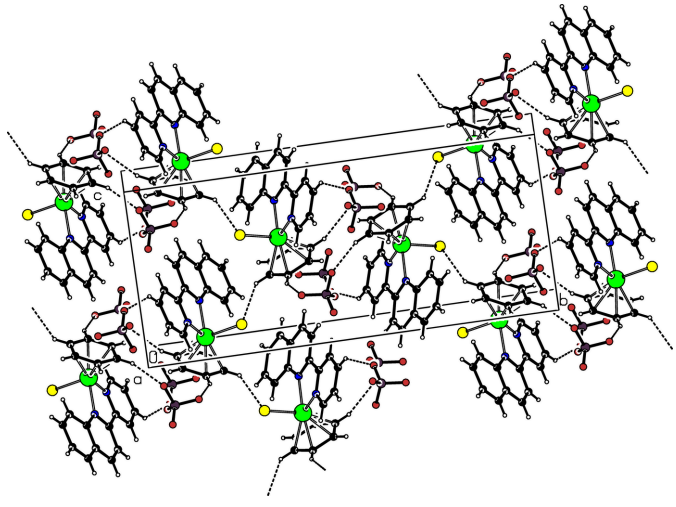


Figure 2
The crystal packing of the title compound. The Ru atoms are represented by green spheres, the Cl atoms by yellow spheres, and the F atoms by red spheres of arbitrary radii.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2025). **10**, x241240 [https://doi.org/10.1107/S2414314624012409]

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Crystal data

$[RuCl(C_6H_6)(C_{14}H_{10}N_2)]BF_4$
M_r = 507.68
Monoclinic, $P2_1/c$
a = 8.4191 (3) Å
b = 23.1476 (9) Å
c = 9.9079 (3) Å
β = 94.709 (3)°
V = 1924.35 (12) Å^3
Z = 4
$F(000)$ = 1008
D_x = 1.752 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4311 reflections
θ = 3.4–28.7°
μ = 1.00 mm^{-1}
T = 293 K
Block, orange
0.65 × 0.50 × 0.41 mm

Data collection

Agilent Xcalibur, Atlas, Gemini diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2012)
T_{min} = 0.507, T_{max} = 0.578
8112 measured reflections
4311 independent reflections
3815 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.7°, θ_{min} = 3.4°
h = −10→11
k = −29→31
l = −13→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.093
S = 1.13
4311 reflections
262 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 2.2897P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.36590 (3)	0.35365 (2)	0.55140 (2)	0.03087 (9)
Cl1	0.48682 (11)	0.26281 (4)	0.60853 (11)	0.0510 (2)
F2	0.0921 (4)	0.5390 (2)	0.8475 (3)	0.1168 (14)
F3	0.1988 (4)	0.60983 (16)	0.7391 (5)	0.1201 (14)
F4	0.3426 (3)	0.53126 (16)	0.7890 (3)	0.0961 (10)
F1	0.1343 (5)	0.53076 (17)	0.6300 (3)	0.1116 (13)
C19	0.3184 (6)	0.3211 (2)	0.3438 (4)	0.0585 (11)
H19	0.342384	0.285320	0.307946	0.070*
N2	0.2831 (3)	0.35589 (11)	0.7506 (3)	0.0313 (5)
N1	0.5548 (3)	0.39139 (12)	0.6693 (3)	0.0353 (6)
C14	0.1411 (4)	0.33333 (14)	0.7897 (3)	0.0335 (7)
C18	0.4281 (5)	0.3648 (2)	0.3419 (4)	0.0543 (10)
H18	0.524933	0.358972	0.305041	0.065*
C9	0.0871 (4)	0.34711 (15)	0.9181 (3)	0.0395 (8)
C11	−0.1533 (4)	0.29144 (18)	0.8644 (4)	0.0514 (10)
H11	−0.251959	0.278213	0.887140	0.062*
C20	0.1737 (5)	0.3286 (2)	0.3972 (4)	0.0630 (12)
H20	0.100838	0.298376	0.395571	0.076*
C2	0.8103 (4)	0.43585 (16)	0.6985 (4)	0.0473 (9)
H2	0.905866	0.445181	0.662876	0.057*
C12	−0.0967 (4)	0.27603 (17)	0.7396 (4)	0.0477 (9)
H12	−0.157907	0.251981	0.680845	0.057*
C5	0.5283 (4)	0.40623 (14)	0.7969 (3)	0.0353 (7)
C3	0.7831 (4)	0.45260 (17)	0.8276 (4)	0.0500 (9)
H3	0.858559	0.474045	0.879990	0.060*
C8	0.1852 (5)	0.38125 (18)	1.0081 (4)	0.0493 (9)
H8	0.151892	0.391143	1.092283	0.059*
C1	0.6957 (4)	0.40530 (16)	0.6226 (4)	0.0430 (8)
H1	0.715866	0.393750	0.535760	0.052*
C13	0.0473 (4)	0.29590 (16)	0.7031 (4)	0.0402 (8)
H13	0.083432	0.284658	0.620893	0.048*
C10	−0.0633 (5)	0.32567 (17)	0.9513 (4)	0.0487 (9)
H10	−0.100441	0.335336	1.034212	0.058*
C6	0.3742 (4)	0.38674 (15)	0.8414 (3)	0.0368 (7)
B1	0.1919 (5)	0.5506 (2)	0.7530 (4)	0.0497 (10)
C15	0.1378 (5)	0.3804 (3)	0.4524 (4)	0.0678 (14)
H15	0.041196	0.384661	0.490554	0.081*
C16	0.2430 (7)	0.4273 (2)	0.4530 (4)	0.0717 (15)
H16	0.216515	0.462854	0.488844	0.086*
C7	0.3287 (5)	0.39968 (17)	0.9715 (4)	0.0462 (9)
H7	0.396377	0.420705	1.031986	0.055*
C4	0.6408 (4)	0.43679 (17)	0.8778 (4)	0.0480 (9)
H4	0.620830	0.446693	0.965746	0.058*
C17	0.3906 (6)	0.4190 (2)	0.3973 (4)	0.0636 (12)
H17	0.463368	0.449282	0.397155	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.03032 (14)	0.03298 (15)	0.02952 (14)	0.00145 (11)	0.00382 (9)	−0.00114 (10)
Cl1	0.0498 (5)	0.0383 (5)	0.0662 (6)	0.0080 (4)	0.0128 (4)	0.0086 (4)
F2	0.083 (2)	0.191 (4)	0.082 (2)	−0.038 (2)	0.0366 (18)	−0.001 (2)
F3	0.093 (2)	0.080 (2)	0.189 (4)	−0.005 (2)	0.020 (3)	−0.010 (3)
F4	0.0582 (16)	0.126 (3)	0.104 (2)	0.0188 (18)	0.0070 (16)	0.032 (2)
F1	0.127 (3)	0.142 (3)	0.0637 (18)	0.040 (2)	−0.0099 (18)	−0.036 (2)
C19	0.081 (3)	0.059 (3)	0.0349 (18)	0.000 (2)	0.0039 (19)	−0.0128 (19)
N2	0.0278 (12)	0.0352 (14)	0.0311 (13)	0.0034 (11)	0.0027 (10)	0.0024 (11)
N1	0.0332 (14)	0.0358 (14)	0.0365 (14)	−0.0014 (12)	−0.0003 (11)	0.0022 (12)
C14	0.0297 (15)	0.0352 (16)	0.0363 (16)	0.0080 (13)	0.0057 (12)	0.0051 (13)
C18	0.047 (2)	0.084 (3)	0.0326 (17)	0.001 (2)	0.0095 (16)	0.0049 (19)
C9	0.0412 (18)	0.0405 (18)	0.0382 (17)	0.0108 (15)	0.0110 (14)	0.0080 (15)
C11	0.0379 (19)	0.055 (2)	0.063 (2)	0.0042 (18)	0.0152 (18)	0.014 (2)
C20	0.055 (2)	0.094 (4)	0.038 (2)	−0.020 (3)	−0.0052 (18)	−0.004 (2)
C2	0.0336 (18)	0.044 (2)	0.064 (2)	−0.0069 (16)	0.0032 (16)	0.0088 (18)
C12	0.0335 (17)	0.051 (2)	0.059 (2)	−0.0013 (16)	0.0058 (16)	0.0022 (18)
C5	0.0346 (16)	0.0353 (16)	0.0354 (16)	0.0029 (14)	−0.0009 (13)	0.0014 (13)
C3	0.0398 (19)	0.047 (2)	0.061 (2)	−0.0090 (17)	−0.0110 (17)	0.0007 (18)
C8	0.058 (2)	0.058 (2)	0.0327 (17)	0.005 (2)	0.0105 (16)	−0.0035 (17)
C1	0.0388 (18)	0.045 (2)	0.0455 (19)	−0.0018 (16)	0.0074 (15)	0.0033 (16)
C13	0.0346 (17)	0.0446 (19)	0.0418 (17)	0.0023 (15)	0.0057 (14)	0.0029 (15)
C10	0.048 (2)	0.051 (2)	0.051 (2)	0.0099 (18)	0.0216 (17)	0.0095 (18)
C6	0.0369 (17)	0.0393 (18)	0.0336 (16)	0.0032 (14)	0.0003 (13)	0.0012 (14)
B1	0.042 (2)	0.068 (3)	0.040 (2)	−0.004 (2)	0.0067 (17)	−0.002 (2)
C15	0.041 (2)	0.117 (4)	0.045 (2)	0.025 (3)	0.0020 (17)	0.019 (3)
C16	0.111 (4)	0.060 (3)	0.042 (2)	0.046 (3)	−0.004 (2)	0.008 (2)
C7	0.052 (2)	0.053 (2)	0.0335 (17)	−0.0034 (18)	0.0034 (15)	−0.0065 (16)
C4	0.047 (2)	0.051 (2)	0.0445 (19)	−0.0037 (18)	−0.0065 (16)	−0.0047 (17)
C17	0.086 (3)	0.055 (3)	0.047 (2)	−0.021 (2)	−0.013 (2)	0.020 (2)

Geometric parameters (Å, º)

Ru1—N1	2.086 (3)	C11—C12	1.407 (5)
Ru1—N2	2.147 (3)	C11—H11	0.9300
Ru1—C17	2.172 (4)	C20—C15	1.361 (8)
Ru1—C15	2.173 (4)	C20—H20	0.9300
Ru1—C16	2.183 (4)	C2—C1	1.371 (5)
Ru1—C19	2.196 (4)	C2—C3	1.373 (6)
Ru1—C18	2.197 (4)	C2—H2	0.9300
Ru1—C20	2.209 (4)	C12—C13	1.373 (5)
Ru1—Cl1	2.3840 (9)	C12—H12	0.9300
F2—B1	1.336 (5)	C5—C4	1.384 (5)
F3—B1	1.381 (6)	C5—C6	1.474 (5)
F4—B1	1.365 (5)	C3—C4	1.384 (5)
F1—B1	1.354 (5)	C3—H3	0.9300

C19—C18	1.371 (6)	C8—C7	1.359 (5)
C19—C20	1.379 (6)	C8—H8	0.9300
C19—H19	0.9300	C1—H1	0.9300
N2—C6	1.340 (4)	C13—H13	0.9300
N2—C14	1.388 (4)	C10—H10	0.9300
N1—C5	1.346 (4)	C6—C7	1.407 (5)
N1—C1	1.347 (4)	C15—C16	1.403 (7)
C14—C13	1.414 (5)	C15—H15	0.9300
C14—C9	1.423 (4)	C16—C17	1.413 (7)
C18—C17	1.416 (6)	C16—H16	0.9300
C18—H18	0.9300	C7—H7	0.9300
C9—C8	1.407 (5)	C4—H4	0.9300
C9—C10	1.423 (5)	C17—H17	0.9300
C11—C10	1.355 (6)		

N1—Ru1—N2	76.42 (10)	C15—C20—C19	119.8 (5)
N1—Ru1—C17	89.37 (14)	C15—C20—Ru1	70.5 (2)
N2—Ru1—C17	133.34 (16)	C19—C20—Ru1	71.2 (2)
N1—Ru1—C15	137.61 (19)	C15—C20—H20	120.1
N2—Ru1—C15	93.82 (13)	C19—C20—H20	120.1
C17—Ru1—C15	67.46 (19)	Ru1—C20—H20	130.9
N1—Ru1—C16	103.56 (17)	C1—C2—C3	119.5 (3)
N2—Ru1—C16	102.37 (14)	C1—C2—H2	120.2
C17—Ru1—C16	37.87 (19)	C3—C2—H2	120.2
C15—Ru1—C16	37.6 (2)	C13—C12—C11	121.1 (4)
N1—Ru1—C19	137.72 (15)	C13—C12—H12	119.5
N2—Ru1—C19	145.23 (14)	C11—C12—H12	119.5
C17—Ru1—C19	66.51 (17)	N1—C5—C4	121.0 (3)
C15—Ru1—C19	65.71 (18)	N1—C5—C6	114.9 (3)
C16—Ru1—C19	78.84 (17)	C4—C5—C6	124.1 (3)
N1—Ru1—C18	104.47 (14)	C2—C3—C4	118.4 (3)
N2—Ru1—C18	170.44 (14)	C2—C3—H3	120.8
C17—Ru1—C18	37.83 (17)	C4—C3—H3	120.8
C15—Ru1—C18	79.07 (16)	C7—C8—C9	119.7 (3)
C16—Ru1—C18	68.10 (17)	C7—C8—H8	120.1
C19—Ru1—C18	36.36 (16)	C9—C8—H8	120.1
N1—Ru1—C20	168.06 (15)	N1—C1—C2	122.4 (3)
N2—Ru1—C20	111.55 (14)	N1—C1—H1	118.8
C17—Ru1—C20	78.70 (17)	C2—C1—H1	118.8
C15—Ru1—C20	36.2 (2)	C12—C13—C14	120.5 (3)
C16—Ru1—C20	66.6 (2)	C12—C13—H13	119.8
C19—Ru1—C20	36.47 (17)	C14—C13—H13	119.8
C18—Ru1—C20	66.14 (16)	C11—C10—C9	121.3 (3)
N1—Ru1—Cl1	86.86 (8)	C11—C10—H10	119.4
N2—Ru1—Cl1	88.14 (7)	C9—C10—H10	119.4
C17—Ru1—Cl1	135.88 (15)	N2—C6—C7	123.0 (3)
C15—Ru1—Cl1	134.61 (17)	N2—C6—C5	115.6 (3)
C16—Ru1—Cl1	166.59 (13)	C7—C6—C5	121.4 (3)

C19—Ru1—Cl1	87.78 (13)	F2—B1—F1	111.3 (4)
C18—Ru1—Cl1	101.40 (12)	F2—B1—F4	112.1 (4)
C20—Ru1—Cl1	101.94 (15)	F1—B1—F4	112.4 (4)
C18—C19—C20	122.0 (4)	F2—B1—F3	107.6 (4)
C18—C19—Ru1	71.9 (2)	F1—B1—F3	105.2 (4)
C20—C19—Ru1	72.3 (2)	F4—B1—F3	107.8 (4)
C18—C19—H19	119.0	C20—C15—C16	121.5 (4)
C20—C19—H19	119.0	C20—C15—Ru1	73.4 (3)
Ru1—C19—H19	129.4	C16—C15—Ru1	71.6 (2)
C6—N2—C14	118.2 (3)	C20—C15—H15	119.2
C6—N2—Ru1	114.8 (2)	C16—C15—H15	119.2
C14—N2—Ru1	126.8 (2)	Ru1—C15—H15	128.1
C5—N1—C1	118.7 (3)	C15—C16—C17	117.9 (4)
C5—N1—Ru1	117.1 (2)	C15—C16—Ru1	70.8 (2)
C1—N1—Ru1	124.0 (2)	C17—C16—Ru1	70.6 (2)
N2—C14—C13	120.8 (3)	C15—C16—H16	121.0
N2—C14—C9	120.7 (3)	C17—C16—H16	121.0
C13—C14—C9	118.4 (3)	Ru1—C16—H16	129.8
C19—C18—C17	118.5 (4)	C8—C7—C6	119.5 (3)
C19—C18—Ru1	71.8 (2)	C8—C7—H7	120.2
C17—C18—Ru1	70.1 (2)	C6—C7—H7	120.2
C19—C18—H18	120.8	C3—C4—C5	120.0 (4)
C17—C18—H18	120.8	C3—C4—H4	120.0
Ru1—C18—H18	129.7	C5—C4—H4	120.0
C8—C9—C14	118.6 (3)	C16—C17—C18	120.2 (4)
C8—C9—C10	122.4 (3)	C16—C17—Ru1	71.5 (2)
C14—C9—C10	119.0 (3)	C18—C17—Ru1	72.1 (2)
C10—C11—C12	119.6 (3)	C16—C17—H17	119.9
C10—C11—H11	120.2	C18—C17—H17	119.9
C12—C11—H11	120.2	Ru1—C17—H17	128.8

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···F4^{i}	0.93	2.48	3.375 (5)	162
C16—H16···F1	0.93	2.24	3.148 (6)	162
C19—H19···Cl1^{ii}	0.93	2.65	3.429 (4)	142

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+2; (ii) *x*, −*y*+1/2, *z*−1/2.