Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chlorido(η^6-*p*-cymene)[6-(2-hydroxyphenyl)-2,2′-bipyridine]ruthenium(II) chloride chloroform solvate

Hao-Fei Zhou,[a,b] Zu-Qiang Bian,[b] Zhi-Wei Liu,[b] Chun-Hui Huang[b] and Yong-Liang Zhao[a]*

[a]College of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot, 010021, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, People's Republic of China
Correspondence e-mail: nmgzyl100@163.com

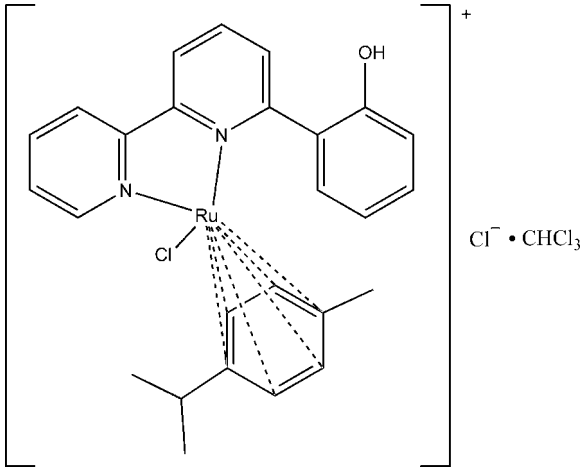
Received 18 April 2007; accepted 15 May 2007

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.026; wR factor = 0.064; data-to-parameter ratio = 18.2.

The title compound, $[RuCl(C_{10}H_{14})(C_{16}H_{12}N_2O)]Cl\cdot CHCl_3$, has been synthesized by the reaction of $[RuCl_2(p\text{-cymene})]_2$ with 6-(2-hydroxyphenyl)-2,2′-bipyridine in acetonitrile. The Ru^{II} cation is in a pseudo-octahedral environment formed by a chloride anion, a cymene molecule (with an η^6 coordination mode) and a chelating 6-(2-hydroxyphenyl)-2,2′-bipyridine ligand. The other chloride anion is uncoordinated but links with the complex *via* O—H···Cl hydrogen bonding. The two methyl groups of the isopropyl group are disordered over two positions in approximately a 0.7:0.3 ratio.

Related literature

For related structures, see: Bardwell *et al.* (1996); Poyatos *et al.* (2004). For synthesis, see: Jeffery *et al.* (1992).



Experimental

Crystal data

$[RuCl(C_{10}H_{14})(C_{16}H_{12}N_2O)]Cl\cdot CHCl_3$
M_r = 673.83
Triclinic, $P\overline{1}$
a = 9.2135 (14) Å
b = 12.8915 (19) Å
c = 13.527 (2) Å
α = 105.406 (3)°
β = 109.022 (2)°
γ = 102.663 (3)°
V = 1379.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 113 (2) K
0.34 × 0.32 × 0.26 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.711, T_{max} = 0.767
12987 measured reflections
6455 independent reflections
5056 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.064
S = 0.99
6455 reflections
354 parameters
48 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—Cl1	2.3924 (6)	Ru1—C19	2.183 (2)
Ru1—N1	2.0706 (16)	Ru1—C20	2.221 (2)
Ru1—N2	2.1209 (16)	Ru1—C21	2.161 (2)
Ru1—C17	2.243 (2)	Ru1—C22	2.192 (2)
Ru1—C18	2.220 (2)		
N1—Ru1—N2	77.00 (6)	N2—Ru1—Cl1	86.47 (4)
N1—Ru1—Cl1	84.07 (5)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Cl2^{i}	0.77 (2)	2.22 (2)	2.9782 (17)	169 (3)

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

The authors thank the National Natural Science Foundation of China (20471004, 20671006 and 20461002) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2245).

References

Bardwell, D. A., Jeffery, J. C. & Ward, M. D. (1996). *Inorg. Chim. Acta*, **241**, 125–129.

Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Jacobson, R. (1998). Private communication to the Rigaku Corporation, Tokyo, Japan.

Jeffery, J. C., Schatz, E. & Ward, M. D. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1921–1927.

Poyatos, M., Mas-Marzá, E., Sanáu, M. & Peris, E. (2004). *Inorg. Chem.* **43**, 1793–1798.

Rigaku (2000). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2005). *CrystalStructure*. Version 3.7.0. Rigaku/MSC, The Woodlands, Texas, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, m1851-m1852 [**doi:10.1107/S1600536807023975**]

Chlorido(η^6-*p*-cymene)[6-(2-hydroxyphenyl)-2,2'-bipyridine]ruthenium(II) chloride chloroform solvate

H.-F. Zhou, Z.-Q. Bian, Z.-W. Liu, C.-H. Huang and Y.-L. Zhao

Comment

The complex consists of $[RuCl(C_{10}H_{14})(C_{16}H_{11}N_2OH)]^+$ cation, the charge being balanced by one interstitial chloride anion. The metal center ruthenium ion is coordinated by a chloride anion, a 6-(2-hydroxyphenyl)-2,2'-bipyridine (hpbipy) ligand linked in a bidentate manner through its two N atoms, defining a five-membered chelate ring, and the arene ring linked through its π-cloud in a η^6 manner (see Fig. 1). The complex crystallizes in the triclinic space group. The geometry around the metal atom is best described as a distorted octahedron, the benzene ring occupying three sites of octahedral co-ordination geometry, the Cl^- anion and the two pyridine N atoms occupying the other three sites of octahedral geometry. The distortion of the octahedral geometry is evident from the values of the N1—Ru1—N2, Cl1—Ru1—N1 and Cl1—Ru1—N2 angles (Table 1). In hpbipy there is a torsion angle of 2.7 (2)° between the two pyridyl rings and there is one of 113.5 (2)° between the central pyridine ring and the phenolate ring, which is typical behavior for mixed pyridine-phenol ligand and occurs because the phenolate lone pair is not in the same plane as the adjacent pyridyl ring (Bardwell *et al.*, 1996). In the other ligand, the *p*-cymene ring is almost planar. The Ru—C distances are almost equal, and Ru to *p*-cymene ring centroid distance agrees well with those found in other (*p*-cymene) ruthenium (II) complexes, for example, $C_{19}H_{26}F_6IN_4PRu$ and $C_{20}H_{28}ClF_6N_4PRu$ described by Poyatos *et al.*, (2004). Defining *X* as the centroid of the arene ring, the Cl1—Ru1-*X*, N1—Ru1-*X* and N2—Ru1-*X* angles are 129.07 (3)°, 128.97 (6)° and 132.85 (5)°, respectively. It is the flexibility of the pyridine ligand that makes possible a near equal distribution of the N, N, and Cl donor atoms around the *p*-cymene ring.

The non-coordinated chloride anion is linked, *via* O—H···Cl hydrogen bonding, with the pyridine-phenol ligand (Table 2 and Fig. 2), leading the parallel supra-molecular chain.

Experimental

6-(2-Hydroxyphenyl)-2,2'-bipyridine (hpbipy) was prepared according to the literature procedure reported by Jeffery *et al.* (1992). The complex was prepared using $[BzRuCl_2]_2$ (0.1225 g, 0.20 mmol) and hpbipy (0.1120 g, 0.23 mmol) dissolved in 50 ml acetonitrile (HPLC grade). The mixture was refluxed with stirring under nitrogen for 10 h. The flask was cooled in an ice bath, a bright orange solid was filtered, washed with small amount of acetonitrile. The solid was dissolved in methanol, then added diethyl ether carefully to get the bright orange precipitate. The precipitate was recrystallized twice yielding bright orange microcrystals (yield 70%). Analysis found: C 51.38%, H 5.28%, N 4.48%; calculated for $[RuCl(C_{10}H_{14})(C_{16}H_{11}N_2OH)]Cl·5H_2O$: C 51.70%, H 5.17%, N 4.64%. TOF-MS: m/*z* = 519 (M—Cl). X-ray quality single crystals were grown by slow evaporation of a $CHCl_3$ solution.

Refinement

Hydroxy H atom was located in a difference Fourier map and refined freely. Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 – 1.00 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for others. The C25 and C26 atoms of isopropyl group were disordered over two positions. The C—C distances of disordered isopropyl group were restrained at 1.54 (1) Å, occupancies were refined to 0.701 (13) and 0.299 (13), respectively.

Figures

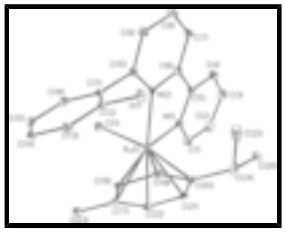


Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 50% probability level. The $CHCl_3$ solvent molecules, the free chloride anion and all H atoms have been omitted for clarity.

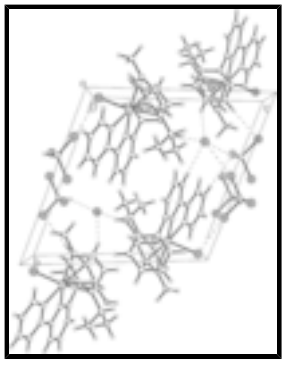


Fig. 2. The crystal structure of the complex, showing the hydrogen bond interactions.

[6-(2-Hydroxyphenyl)-2,2'-bipyridine]chloro(η^6-*p*-cymene)ruthenium(II) chloride chloroform solvate

Crystal data

$[RuCl(C_{10}H_{14})(C_{16}H_{12}N_2O)]Cl·CHCl_3$	Z = 2
M_r = 673.83	F_{000} = 680
Triclinic, $P\overline{1}$	D_x = 1.622 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71070 Å
a = 9.2135 (14) Å	Cell parameters from 4697 reflections
b = 12.8915 (19) Å	θ = 1.7–27.9º
c = 13.527 (2) Å	μ = 1.08 mm^{-1}
α = 105.406 (3)º	T = 113 (2) K
β = 109.022 (2)º	Block, orange
γ = 102.663 (3)º	0.34 × 0.32 × 0.26 mm
V = 1379.4 (4) Å^3	

Data collection

Rigaku Saturn diffractometer	6455 independent reflections
Radiation source: rotating anode	5056 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.032$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 27.9^{o}$
$T = 113(2)$ K	$\theta_{min} = 1.7^{o}$
ω scans	$h = -11 \rightarrow 12$
Absorption correction: multi-scan (Jacobson, 1998)	$k = -16 \rightarrow 13$
$T_{min} = 0.711$, $T_{max} = 0.767$	$l = -17 \rightarrow 17$
12987 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} = 0.003$
6455 reflections	$\Delta\rho_{max} = 0.50$ e $Å^{-3}$
354 parameters	$\Delta\rho_{min} = -0.53$ e $Å^{-3}$
48 restraints	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0062 (5)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ru1	0.06609 (2)	0.119648 (12)	0.263140 (13)	0.01230 (6)	

Cl1	−0.13959 (6)	0.04881 (4)	0.07590 (4)	0.01967 (12)
Cl2	0.77785 (6)	0.28443 (4)	0.72438 (4)	0.01802 (11)
Cl3	0.77344 (8)	0.26543 (5)	1.01892 (4)	0.03189 (15)
Cl4	0.52444 (8)	0.35538 (5)	0.92069 (6)	0.03474 (15)
Cl5	0.85304 (9)	0.50928 (5)	1.06956 (5)	0.03829 (17)
O1	−0.11761 (19)	0.25455 (12)	0.53521 (12)	0.0195 (3)
H1	−0.135 (3)	0.260 (2)	0.588 (2)	0.035 (8)*
N1	0.1906 (2)	0.22880 (13)	0.20732 (13)	0.0141 (3)
N2	−0.0190 (2)	0.26007 (12)	0.29346 (12)	0.0111 (3)
C1	0.2867 (3)	0.20021 (18)	0.15562 (16)	0.0192 (4)
H1A	0.2904	0.1247	0.1376	0.023*
C2	0.3796 (3)	0.27783 (18)	0.12835 (17)	0.0232 (5)
H2	0.4485	0.2566	0.0935	0.028*
C3	0.3715 (3)	0.38664 (18)	0.15209 (17)	0.0229 (5)
H3	0.4359	0.4415	0.1347	0.027*
C4	0.2684 (3)	0.41545 (17)	0.20171 (16)	0.0184 (4)
H4	0.2589	0.4894	0.2167	0.022*
C5	0.1793 (2)	0.33424 (15)	0.22897 (15)	0.0137 (4)
C6	0.0646 (2)	0.35315 (15)	0.27995 (15)	0.0124 (4)
C7	0.0400 (3)	0.45734 (16)	0.31050 (16)	0.0164 (4)
H7	0.1024	0.5214	0.3027	0.020*
C8	−0.0764 (3)	0.46652 (17)	0.35239 (17)	0.0200 (5)
H8	−0.0935	0.5375	0.3757	0.024*
C9	−0.1676 (3)	0.37102 (16)	0.35989 (17)	0.0178 (4)
H9	−0.2514	0.3754	0.3855	0.021*
C10	−0.1381 (2)	0.26836 (15)	0.33020 (15)	0.0135 (4)
C11	−0.2399 (2)	0.16594 (15)	0.33706 (16)	0.0134 (4)
C12	−0.2287 (2)	0.16362 (16)	0.44268 (16)	0.0141 (4)
C13	−0.3235 (3)	0.06753 (16)	0.44986 (17)	0.0177 (4)
H13	−0.3146	0.0653	0.5212	0.021*
C14	−0.4304 (3)	−0.02437 (16)	0.35292 (18)	0.0192 (4)
H14	−0.4944	−0.0898	0.3579	0.023*
C15	−0.4449 (3)	−0.02147 (16)	0.24794 (18)	0.0197 (5)
H15	−0.5195	−0.0844	0.1816	0.024*
C16	−0.3505 (3)	0.07302 (16)	0.24032 (17)	0.0168 (4)
H16	−0.3611	0.0747	0.1686	0.020*
C17	0.0212 (3)	−0.06009 (17)	0.25867 (19)	0.0227 (5)
C18	−0.0163 (3)	0.00294 (16)	0.34352 (18)	0.0200 (5)
H18	−0.1196	−0.0250	0.3451	0.024*
C19	0.0996 (3)	0.10807 (17)	0.42677 (17)	0.0179 (4)
H19	0.0708	0.1497	0.4824	0.021*
C20	0.2566 (2)	0.15333 (16)	0.43013 (17)	0.0160 (4)
C21	0.2889 (3)	0.08878 (16)	0.34213 (17)	0.0174 (4)
H21	0.3912	0.1169	0.3393	0.021*
C22	0.1741 (3)	−0.01612 (17)	0.25820 (18)	0.0202 (5)
H22	0.2011	−0.0570	0.2011	0.024*
C23	−0.1038 (3)	−0.16856 (17)	0.1673 (2)	0.0352 (6)
H23A	−0.0809	−0.1818	0.1000	0.053*
H23B	−0.2126	−0.1620	0.1496	0.053*

H23C	−0.0995	−0.2327	0.1927	0.053*	
C24	0.3834 (3)	0.26317 (17)	0.52252 (17)	0.0221 (5)	
H24A	0.4505	0.2432	0.5804	0.026*	0.701 (13)
H24B	0.4704	0.2383	0.5583	0.026*	0.299 (13)
C25	0.3058 (5)	0.3461 (4)	0.5771 (4)	0.0319 (13)	0.701 (13)
H25A	0.2449	0.3092	0.6130	0.048*	0.701 (13)
H25B	0.2317	0.3643	0.5188	0.048*	0.701 (13)
H25C	0.3922	0.4166	0.6335	0.048*	0.701 (13)
C26	0.4940 (8)	0.3301 (5)	0.4811 (6)	0.0210 (12)	0.701 (13)
H26A	0.4284	0.3535	0.4236	0.031*	0.701 (13)
H26B	0.5481	0.2817	0.4490	0.031*	0.701 (13)
H26C	0.5763	0.3980	0.5443	0.031*	0.701 (13)
C25'	0.3291 (14)	0.3035 (12)	0.6121 (10)	0.042 (3)	0.299 (13)
H25D	0.4173	0.3694	0.6742	0.063*	0.299 (13)
H25E	0.3001	0.2421	0.6393	0.063*	0.299 (13)
H25F	0.2337	0.3260	0.5825	0.063*	0.299 (13)
C26'	0.461 (2)	0.3468 (13)	0.4826 (16)	0.032 (4)	0.299 (13)
H26D	0.3882	0.3888	0.4585	0.048*	0.299 (13)
H26E	0.4821	0.3065	0.4192	0.048*	0.299 (13)
H26F	0.5641	0.4005	0.5437	0.048*	0.299 (13)
C27	0.7341 (3)	0.37268 (17)	0.96670 (17)	0.0221 (5)	
H27	0.7638	0.3645	0.9009	0.027*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01053 (9)	0.00951 (8)	0.01572 (9)	0.00345 (6)	0.00411 (6)	0.00437 (6)
Cl1	0.0179 (3)	0.0177 (2)	0.0158 (2)	0.00578 (19)	0.0030 (2)	−0.00029 (18)
Cl2	0.0196 (3)	0.0158 (2)	0.0172 (2)	0.00279 (19)	0.0078 (2)	0.00601 (18)
Cl3	0.0382 (4)	0.0201 (3)	0.0211 (3)	0.0056 (2)	−0.0036 (2)	0.0061 (2)
Cl4	0.0265 (3)	0.0342 (3)	0.0495 (4)	0.0095 (3)	0.0160 (3)	0.0240 (3)
Cl5	0.0524 (5)	0.0186 (3)	0.0234 (3)	−0.0026 (3)	0.0025 (3)	0.0049 (2)
O1	0.0203 (9)	0.0178 (8)	0.0148 (8)	−0.0013 (6)	0.0077 (7)	0.0033 (6)
N1	0.0145 (9)	0.0141 (8)	0.0118 (8)	0.0038 (7)	0.0044 (7)	0.0040 (6)
N2	0.0110 (8)	0.0087 (7)	0.0085 (7)	0.0011 (6)	0.0010 (6)	0.0010 (6)
C1	0.0214 (12)	0.0214 (10)	0.0148 (10)	0.0092 (9)	0.0076 (9)	0.0045 (8)
C2	0.0267 (13)	0.0269 (11)	0.0184 (11)	0.0086 (9)	0.0129 (10)	0.0078 (9)
C3	0.0227 (12)	0.0279 (12)	0.0221 (11)	0.0048 (9)	0.0128 (10)	0.0135 (9)
C4	0.0221 (12)	0.0162 (10)	0.0178 (10)	0.0052 (8)	0.0085 (9)	0.0080 (8)
C5	0.0151 (10)	0.0137 (9)	0.0100 (9)	0.0037 (8)	0.0037 (8)	0.0035 (7)
C6	0.0132 (10)	0.0124 (9)	0.0107 (9)	0.0038 (7)	0.0034 (8)	0.0054 (7)
C7	0.0196 (11)	0.0123 (9)	0.0150 (10)	0.0023 (8)	0.0056 (8)	0.0062 (7)
C8	0.0256 (12)	0.0125 (10)	0.0228 (11)	0.0081 (8)	0.0114 (10)	0.0046 (8)
C9	0.0211 (12)	0.0150 (10)	0.0216 (11)	0.0072 (8)	0.0128 (9)	0.0070 (8)
C10	0.0140 (10)	0.0124 (9)	0.0118 (9)	0.0034 (7)	0.0041 (8)	0.0035 (7)
C11	0.0108 (10)	0.0103 (9)	0.0192 (10)	0.0045 (7)	0.0063 (8)	0.0047 (7)
C12	0.0118 (10)	0.0129 (9)	0.0182 (10)	0.0050 (7)	0.0066 (8)	0.0054 (8)
C13	0.0179 (11)	0.0163 (10)	0.0244 (11)	0.0076 (8)	0.0112 (9)	0.0110 (8)

C14	0.0117 (11)	0.0119 (10)	0.0381 (12)	0.0040 (8)	0.0132 (10)	0.0114 (9)
C15	0.0109 (10)	0.0123 (9)	0.0275 (11)	0.0033 (8)	0.0044 (9)	−0.0006 (8)
C16	0.0135 (10)	0.0174 (10)	0.0208 (10)	0.0070 (8)	0.0082 (9)	0.0058 (8)
C17	0.0170 (11)	0.0119 (10)	0.0364 (13)	0.0056 (8)	0.0047 (10)	0.0118 (9)
C18	0.0136 (11)	0.0181 (10)	0.0356 (12)	0.0068 (8)	0.0101 (10)	0.0196 (9)
C19	0.0174 (11)	0.0223 (10)	0.0199 (10)	0.0095 (8)	0.0075 (9)	0.0146 (8)
C20	0.0119 (10)	0.0187 (10)	0.0191 (10)	0.0065 (8)	0.0032 (8)	0.0123 (8)
C21	0.0114 (10)	0.0175 (10)	0.0278 (11)	0.0085 (8)	0.0073 (9)	0.0129 (8)
C22	0.0190 (12)	0.0144 (10)	0.0304 (12)	0.0118 (8)	0.0098 (10)	0.0085 (9)
C23	0.0208 (13)	0.0124 (10)	0.0574 (17)	0.0045 (9)	0.0029 (12)	0.0075 (10)
C24	0.0122 (11)	0.0286 (12)	0.0180 (11)	0.0029 (9)	0.0013 (9)	0.0066 (9)
C25	0.025 (2)	0.032 (2)	0.024 (2)	0.0016 (16)	0.0100 (16)	−0.0058 (16)
C26	0.021 (2)	0.012 (2)	0.025 (2)	0.0019 (17)	0.0072 (18)	0.0045 (18)
C25'	0.028 (5)	0.035 (5)	0.033 (5)	−0.004 (4)	0.004 (4)	−0.010 (4)
C26'	0.048 (8)	0.011 (5)	0.023 (5)	0.009 (4)	0.003 (5)	0.000 (4)
C27	0.0254 (13)	0.0185 (10)	0.0179 (10)	0.0041 (9)	0.0057 (9)	0.0064 (8)

Geometric parameters (Å, °)

Ru1—Cl1	2.3924 (6)	C14—C15	1.394 (3)
Ru1—N1	2.0706 (16)	C14—H14	0.9500
Ru1—N2	2.1209 (16)	C15—C16	1.382 (3)
Ru1—C17	2.243 (2)	C15—H15	0.9500
Ru1—C18	2.220 (2)	C16—H16	0.9500
Ru1—C19	2.183 (2)	C17—C22	1.402 (3)
Ru1—C20	2.221 (2)	C17—C18	1.408 (3)
Ru1—C21	2.161 (2)	C17—C23	1.502 (3)
Ru1—C22	2.192 (2)	C18—C19	1.420 (3)
Cl3—C27	1.765 (2)	C18—H18	0.9500
Cl4—C27	1.767 (2)	C19—C20	1.417 (3)
Cl5—C27	1.760 (2)	C19—H19	0.9500
O1—C12	1.359 (2)	C20—C21	1.418 (3)
O1—H1	0.77 (2)	C20—C24	1.521 (3)
N1—C5	1.347 (2)	C21—C22	1.418 (3)
N1—C1	1.349 (3)	C21—H21	0.9500
N2—C10	1.356 (2)	C22—H22	0.9500
N2—C6	1.367 (2)	C23—H23A	0.9800
C1—C2	1.377 (3)	C23—H23B	0.9800
C1—H1A	0.9500	C23—H23C	0.9800
C2—C3	1.378 (3)	C24—C25'	1.471 (7)
C2—H2	0.9500	C24—C26'	1.479 (8)
C3—C4	1.389 (3)	C24—C26	1.529 (4)
C3—H3	0.9500	C24—C25	1.569 (4)
C4—C5	1.389 (3)	C24—H24A	0.9601
C4—H4	0.9500	C24—H24B	0.9600
C5—C6	1.467 (3)	C25—H25A	0.9800
C6—C7	1.388 (3)	C25—H25B	0.9800
C7—C8	1.379 (3)	C25—H25C	0.9800
C7—H7	0.9500	C26—H26A	0.9800

C8—C9	1.379 (3)	C26—H26B	0.9800
C8—H8	0.9500	C26—H26C	0.9800
C9—C10	1.391 (3)	C25'—H25D	0.9800
C9—H9	0.9500	C25'—H25E	0.9800
C10—C11	1.487 (3)	C25'—H25F	0.9800
C11—C16	1.396 (3)	C26'—H26D	0.9800
C11—C12	1.407 (3)	C26'—H26E	0.9800
C12—C13	1.397 (3)	C26'—H26F	0.9800
C13—C14	1.384 (3)	C27—H27	1.0000
C13—H13	0.9500		
N1—Ru1—N2	77.00 (6)	C15—C16—C11	120.62 (19)
N1—Ru1—C21	88.96 (7)	C15—C16—H16	119.7
N2—Ru1—C21	135.12 (7)	C11—C16—H16	119.7
N1—Ru1—C19	134.95 (7)	C22—C17—C18	118.48 (19)
N2—Ru1—C19	93.42 (7)	C22—C17—C23	121.0 (2)
C21—Ru1—C19	67.04 (8)	C18—C17—C23	120.5 (2)
N1—Ru1—C22	105.25 (7)	C22—C17—Ru1	69.58 (11)
N2—Ru1—C22	171.71 (7)	C18—C17—Ru1	70.72 (11)
C21—Ru1—C22	38.02 (7)	C23—C17—Ru1	128.70 (16)
C19—Ru1—C22	79.32 (8)	C17—C18—C19	120.3 (2)
N1—Ru1—C18	168.10 (7)	C17—C18—Ru1	72.51 (12)
N2—Ru1—C18	110.11 (7)	C19—C18—Ru1	69.79 (11)
C21—Ru1—C18	79.28 (8)	C17—C18—H18	119.9
C19—Ru1—C18	37.61 (7)	C19—C18—H18	119.9
C22—Ru1—C18	66.35 (8)	Ru1—C18—H18	130.5
N1—Ru1—C20	101.30 (7)	C20—C19—C18	122.55 (19)
N2—Ru1—C20	103.22 (7)	C20—C19—Ru1	72.67 (11)
C21—Ru1—C20	37.73 (7)	C18—C19—Ru1	72.60 (12)
C19—Ru1—C20	37.54 (7)	C20—C19—H19	118.7
C22—Ru1—C20	68.57 (8)	C18—C19—H19	118.7
C18—Ru1—C20	68.15 (8)	Ru1—C19—H19	128.4
N1—Ru1—C17	138.90 (7)	C19—C20—C21	115.58 (18)
N2—Ru1—C17	143.16 (7)	C19—C20—C24	122.46 (18)
C21—Ru1—C17	67.55 (8)	C21—C20—C24	121.96 (18)
C19—Ru1—C17	67.27 (8)	C19—C20—Ru1	69.79 (12)
C22—Ru1—C17	36.82 (8)	C21—C20—Ru1	68.83 (11)
C18—Ru1—C17	36.77 (7)	C24—C20—Ru1	132.06 (14)
C20—Ru1—C17	80.77 (8)	C20—C21—C22	122.46 (19)
N1—Ru1—Cl1	84.07 (5)	C20—C21—Ru1	73.44 (12)
N2—Ru1—Cl1	86.47 (4)	C22—C21—Ru1	72.18 (12)
C21—Ru1—Cl1	134.78 (5)	C20—C21—H21	118.8
C19—Ru1—Cl1	139.91 (6)	C22—C21—H21	118.8
C22—Ru1—Cl1	101.66 (6)	Ru1—C21—H21	127.9
C18—Ru1—Cl1	105.53 (6)	C17—C22—C21	120.62 (19)
C20—Ru1—Cl1	169.72 (5)	C17—C22—Ru1	73.59 (12)
C17—Ru1—Cl1	89.41 (6)	C21—C22—Ru1	69.80 (11)
C12—O1—H1	114 (2)	C17—C22—H22	119.7
C5—N1—C1	119.58 (17)	C21—C22—H22	119.7
C5—N1—Ru1	117.58 (13)	Ru1—C22—H22	129.3

C1—N1—Ru1	122.77 (13)	C17—C23—H23A	109.5
C10—N2—C6	118.36 (16)	C17—C23—H23B	109.5
C10—N2—Ru1	127.07 (12)	H23A—C23—H23B	109.5
C6—N2—Ru1	114.45 (13)	C17—C23—H23C	109.5
N1—C1—C2	121.60 (19)	H23A—C23—H23C	109.5
N1—C1—H1A	119.2	H23B—C23—H23C	109.5
C2—C1—H1A	119.2	C25'—C24—C26'	119.1 (7)
C1—C2—C3	119.3 (2)	C25'—C24—C20	111.0 (4)
C1—C2—H2	120.3	C26'—C24—C20	114.9 (8)
C3—C2—H2	120.3	C25'—C24—C26	130.3 (6)
C2—C3—C4	119.4 (2)	C20—C24—C26	112.7 (3)
C2—C3—H3	120.3	C26'—C24—C25	92.8 (6)
C4—C3—H3	120.3	C20—C24—C25	112.8 (2)
C3—C4—C5	118.83 (19)	C26—C24—C25	107.2 (3)
C3—C4—H4	120.6	C25'—C24—H24A	79.2
C5—C4—H4	120.6	C26'—C24—H24A	119.5
N1—C5—C4	121.24 (18)	C20—C24—H24A	108.0
N1—C5—C6	114.50 (16)	C26—C24—H24A	108.0
C4—C5—C6	124.24 (18)	C25—C24—H24A	107.9
N2—C6—C7	122.16 (18)	C25'—C24—H24B	102.7
N2—C6—C5	115.25 (16)	C26'—C24—H24B	103.4
C7—C6—C5	122.58 (17)	C20—C24—H24B	103.2
C8—C7—C6	119.05 (18)	C26—C24—H24B	89.4
C8—C7—H7	120.5	C25—C24—H24B	129.2
C6—C7—H7	120.5	C24—C25—H25A	109.5
C9—C8—C7	118.88 (18)	C24—C25—H25B	109.5
C9—C8—H8	120.6	C24—C25—H25C	109.5
C7—C8—H8	120.6	C24—C26—H26A	109.5
C8—C9—C10	120.56 (19)	C24—C26—H26B	109.5
C8—C9—H9	119.7	C24—C26—H26C	109.5
C10—C9—H9	119.7	C24—C25'—H25D	109.5
N2—C10—C9	120.80 (17)	C24—C25'—H25E	109.5
N2—C10—C11	119.58 (16)	H25D—C25'—H25E	109.5
C9—C10—C11	119.61 (18)	C24—C25'—H25F	109.5
C16—C11—C12	119.10 (18)	H25D—C25'—H25F	109.5
C16—C11—C10	121.23 (18)	H25E—C25'—H25F	109.5
C12—C11—C10	119.64 (17)	C24—C26'—H26D	109.5
O1—C12—C13	122.38 (18)	C24—C26'—H26E	109.5
O1—C12—C11	117.55 (17)	H26D—C26'—H26E	109.5
C13—C12—C11	119.98 (18)	C24—C26'—H26F	109.5
C14—C13—C12	119.89 (19)	H26D—C26'—H26F	109.5
C14—C13—H13	120.1	H26E—C26'—H26F	109.5
C12—C13—H13	120.1	Cl5—C27—Cl3	110.73 (12)
C13—C14—C15	120.39 (18)	Cl5—C27—Cl4	110.80 (12)
C13—C14—H14	119.8	Cl3—C27—Cl4	110.02 (12)
C15—C14—H14	119.8	Cl5—C27—H27	108.4
C16—C15—C14	119.99 (18)	Cl3—C27—H27	108.4
C16—C15—H15	120.0	Cl4—C27—H27	108.4
C14—C15—H15	120.0		

N2—Ru1—N1—C5	8.66 (13)	C22—Ru1—C18—C17	−29.09 (13)
C21—Ru1—N1—C5	−128.35 (15)	C20—Ru1—C18—C17	−104.36 (14)
C19—Ru1—N1—C5	−73.06 (17)	Cl1—Ru1—C18—C17	67.07 (13)
C22—Ru1—N1—C5	−163.10 (14)	N1—Ru1—C18—C19	56.9 (4)
C18—Ru1—N1—C5	−119.3 (3)	N2—Ru1—C18—C19	−68.20 (13)
C20—Ru1—N1—C5	−92.48 (15)	C21—Ru1—C18—C19	66.12 (13)
C17—Ru1—N1—C5	178.64 (13)	C22—Ru1—C18—C19	103.71 (14)
Cl1—Ru1—N1—C5	96.39 (14)	C20—Ru1—C18—C19	28.43 (12)
N2—Ru1—N1—C1	−174.45 (17)	C17—Ru1—C18—C19	132.79 (19)
C21—Ru1—N1—C1	48.54 (17)	Cl1—Ru1—C18—C19	−160.13 (11)
C19—Ru1—N1—C1	103.83 (17)	C17—C18—C19—C20	−1.1 (3)
C22—Ru1—N1—C1	13.79 (18)	Ru1—C18—C19—C20	−55.23 (17)
C18—Ru1—N1—C1	57.6 (4)	C17—C18—C19—Ru1	54.14 (17)
C20—Ru1—N1—C1	84.41 (17)	N1—Ru1—C19—C20	−32.36 (16)
C17—Ru1—N1—C1	−4.5 (2)	N2—Ru1—C19—C20	−107.36 (12)
Cl1—Ru1—N1—C1	−86.72 (16)	C21—Ru1—C19—C20	30.85 (11)
N1—Ru1—N2—C10	174.27 (16)	C22—Ru1—C19—C20	68.59 (12)
C21—Ru1—N2—C10	−110.70 (17)	C18—Ru1—C19—C20	133.50 (18)
C19—Ru1—N2—C10	−50.29 (16)	C17—Ru1—C19—C20	105.06 (13)
C18—Ru1—N2—C10	−15.70 (17)	Cl1—Ru1—C19—C20	164.07 (9)
C20—Ru1—N2—C10	−86.97 (16)	N1—Ru1—C19—C18	−165.86 (11)
C17—Ru1—N2—C10	5.3 (2)	N2—Ru1—C19—C18	119.14 (12)
Cl1—Ru1—N2—C10	89.55 (15)	C21—Ru1—C19—C18	−102.65 (13)
N1—Ru1—N2—C6	−9.87 (13)	C22—Ru1—C19—C18	−64.91 (13)
C21—Ru1—N2—C6	65.17 (16)	C20—Ru1—C19—C18	−133.50 (18)
C19—Ru1—N2—C6	125.57 (14)	C17—Ru1—C19—C18	−28.44 (12)
C18—Ru1—N2—C6	160.16 (13)	Cl1—Ru1—C19—C18	30.57 (16)
C20—Ru1—N2—C6	88.90 (14)	C18—C19—C20—C21	2.3 (3)
C17—Ru1—N2—C6	−178.87 (13)	Ru1—C19—C20—C21	−52.92 (15)
Cl1—Ru1—N2—C6	−94.59 (13)	C18—C19—C20—C24	−177.07 (19)
C5—N1—C1—C2	2.8 (3)	Ru1—C19—C20—C24	127.73 (18)
Ru1—N1—C1—C2	−174.08 (16)	C18—C19—C20—Ru1	55.20 (18)
N1—C1—C2—C3	−1.5 (3)	N1—Ru1—C20—C19	157.28 (12)
C1—C2—C3—C4	−0.8 (3)	N2—Ru1—C20—C19	78.16 (12)
C2—C3—C4—C5	1.8 (3)	C21—Ru1—C20—C19	−129.49 (17)
C1—N1—C5—C4	−1.7 (3)	C22—Ru1—C20—C19	−100.62 (13)
Ru1—N1—C5—C4	175.28 (15)	C18—Ru1—C20—C19	−28.48 (11)
C1—N1—C5—C6	176.91 (18)	C17—Ru1—C20—C19	−64.47 (12)
Ru1—N1—C5—C6	−6.1 (2)	Cl1—Ru1—C20—C19	−82.0 (3)
C3—C4—C5—N1	−0.5 (3)	N1—Ru1—C20—C21	−73.23 (12)
C3—C4—C5—C6	−179.03 (19)	N2—Ru1—C20—C21	−152.35 (11)
C10—N2—C6—C7	5.0 (3)	C19—Ru1—C20—C21	129.49 (17)
Ru1—N2—C6—C7	−171.30 (15)	C22—Ru1—C20—C21	28.87 (12)
C10—N2—C6—C5	−173.88 (16)	C18—Ru1—C20—C21	101.01 (13)
Ru1—N2—C6—C5	9.9 (2)	C17—Ru1—C20—C21	65.02 (12)
N1—C5—C6—N2	−2.7 (2)	Cl1—Ru1—C20—C21	47.5 (4)
C4—C5—C6—N2	175.84 (18)	N1—Ru1—C20—C24	41.3 (2)
N1—C5—C6—C7	178.44 (18)	N2—Ru1—C20—C24	−37.8 (2)
C4—C5—C6—C7	−3.0 (3)	C21—Ru1—C20—C24	114.5 (2)

N2—C6—C7—C8	−2.2 (3)	C19—Ru1—C20—C24	−116.0 (2)
C5—C6—C7—C8	176.54 (19)	C22—Ru1—C20—C24	143.4 (2)
C6—C7—C8—C9	−1.7 (3)	C18—Ru1—C20—C24	−144.5 (2)
C7—C8—C9—C10	2.7 (3)	C17—Ru1—C20—C24	179.5 (2)
C6—N2—C10—C9	−3.8 (3)	Cl1—Ru1—C20—C24	162.0 (2)
Ru1—N2—C10—C9	171.88 (14)	C19—C20—C21—C22	−2.0 (3)
C6—N2—C10—C11	175.17 (17)	C24—C20—C21—C22	177.34 (19)
Ru1—N2—C10—C11	−9.1 (3)	Ru1—C20—C21—C22	−55.43 (18)
C8—C9—C10—N2	0.1 (3)	C19—C20—C21—Ru1	53.41 (16)
C8—C9—C10—C11	−178.93 (19)	C24—C20—C21—Ru1	−127.24 (18)
N2—C10—C11—C16	−68.5 (3)	N1—Ru1—C21—C20	110.11 (12)
C9—C10—C11—C16	110.6 (2)	N2—Ru1—C21—C20	39.81 (15)
N2—C10—C11—C12	113.5 (2)	C19—Ru1—C21—C20	−30.71 (11)
C9—C10—C11—C12	−67.5 (3)	C22—Ru1—C21—C20	−133.13 (18)
C16—C11—C12—O1	178.79 (18)	C18—Ru1—C21—C20	−68.01 (12)
C10—C11—C12—O1	−3.2 (3)	C17—Ru1—C21—C20	−104.51 (13)
C16—C11—C12—C13	2.2 (3)	Cl1—Ru1—C21—C20	−169.31 (9)
C10—C11—C12—C13	−179.74 (19)	N1—Ru1—C21—C22	−116.76 (13)
O1—C12—C13—C14	−177.60 (18)	N2—Ru1—C21—C22	172.94 (11)
C11—C12—C13—C14	−1.2 (3)	C19—Ru1—C21—C22	102.43 (14)
C12—C13—C14—C15	−0.3 (3)	C18—Ru1—C21—C22	65.12 (13)
C13—C14—C15—C16	0.8 (3)	C20—Ru1—C21—C22	133.13 (18)
C14—C15—C16—C11	0.2 (3)	C17—Ru1—C21—C22	28.62 (12)
C12—C11—C16—C15	−1.7 (3)	Cl1—Ru1—C21—C22	−36.18 (15)
C10—C11—C16—C15	−179.75 (19)	C18—C17—C22—C21	0.7 (3)
N1—Ru1—C17—C22	30.28 (18)	C23—C17—C22—C21	177.4 (2)
N2—Ru1—C17—C22	−166.14 (12)	Ru1—C17—C22—C21	53.67 (17)
C21—Ru1—C17—C22	−29.49 (12)	C18—C17—C22—Ru1	−52.93 (17)
C19—Ru1—C17—C22	−102.96 (14)	C23—C17—C22—Ru1	123.7 (2)
C18—Ru1—C17—C22	−132.01 (19)	C20—C21—C22—C17	0.6 (3)
C20—Ru1—C17—C22	−66.37 (13)	Ru1—C21—C22—C17	−55.43 (18)
Cl1—Ru1—C17—C22	110.55 (12)	C20—C21—C22—Ru1	56.00 (17)
N1—Ru1—C17—C18	162.29 (12)	N1—Ru1—C22—C17	−159.91 (12)
N2—Ru1—C17—C18	−34.14 (18)	C21—Ru1—C22—C17	132.38 (19)
C21—Ru1—C17—C18	102.51 (14)	C19—Ru1—C22—C17	66.16 (13)
C19—Ru1—C17—C18	29.05 (12)	C18—Ru1—C22—C17	29.05 (12)
C22—Ru1—C17—C18	132.01 (19)	C20—Ru1—C22—C17	103.71 (14)
C20—Ru1—C17—C18	65.63 (13)	Cl1—Ru1—C22—C17	−72.95 (13)
Cl1—Ru1—C17—C18	−117.45 (12)	N1—Ru1—C22—C21	67.72 (13)
N1—Ru1—C17—C23	−83.6 (2)	C19—Ru1—C22—C21	−66.21 (13)
N2—Ru1—C17—C23	79.9 (2)	C18—Ru1—C22—C21	−103.32 (14)
C21—Ru1—C17—C23	−143.4 (2)	C20—Ru1—C22—C21	−28.67 (12)
C19—Ru1—C17—C23	143.1 (2)	C17—Ru1—C22—C21	−132.38 (19)
C22—Ru1—C17—C23	−113.9 (3)	Cl1—Ru1—C22—C21	154.67 (11)
C18—Ru1—C17—C23	114.1 (3)	C19—C20—C24—C25'	8.1 (9)
C20—Ru1—C17—C23	179.7 (2)	C21—C20—C24—C25'	−171.2 (9)
Cl1—Ru1—C17—C23	−3.4 (2)	Ru1—C20—C24—C25'	99.4 (9)
C22—C17—C18—C19	−0.5 (3)	C19—C20—C24—C26'	−130.7 (8)
C23—C17—C18—C19	−177.12 (19)	C21—C20—C24—C26'	50.0 (8)

Ru1—C17—C18—C19	−52.88 (17)	Ru1—C20—C24—C26'	−39.4 (8)
C22—C17—C18—Ru1	52.40 (17)	C19—C20—C24—C26	−147.6 (3)
C23—C17—C18—Ru1	−124.2 (2)	C21—C20—C24—C26	33.1 (4)
N1—Ru1—C18—C17	−75.9 (3)	Ru1—C20—C24—C26	−56.3 (4)
N2—Ru1—C18—C17	159.00 (12)	C19—C20—C24—C25	−26.0 (4)
C21—Ru1—C18—C17	−66.68 (13)	C21—C20—C24—C25	154.7 (3)
C19—Ru1—C18—C17	−132.79 (19)	Ru1—C20—C24—C25	65.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···Cl2^{i}	0.77 (2)	2.22 (2)	2.9782 (17)	169 (3)

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

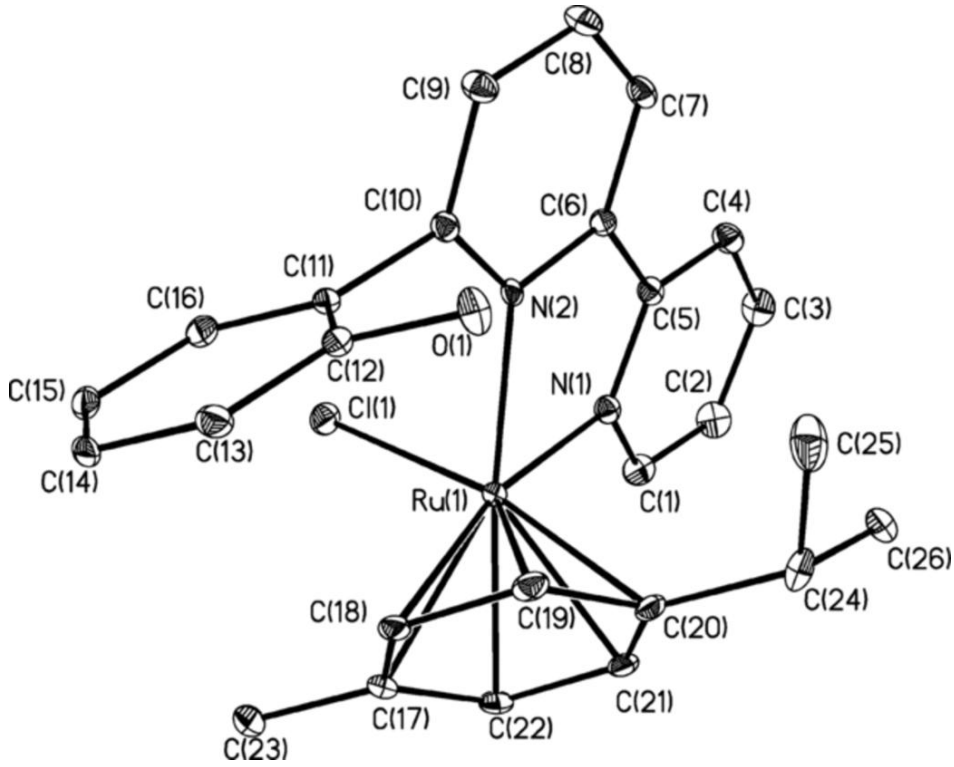

C(8)
C(9)
C(7)
C(10)
C(6)
C(4)
C(11)
C(16)
N(2)
C(5)
C(3)
O(1)
C(12)
C(15)
N(1)
C(2)
Cl(1)
C(25)
C(13)
C(14)
Ru(1)
C(1)
C(26)
C(24)
C(18)
C(19)
C(20)
C(21)
C(17)
C(22)
C(23)

Fig. 2