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# $(\eta^6\text{-Benzene})(2,2'\text{-bipyridine-}\kappa^2\text{N,N}')\text{-chloridoruthenium(II) chloride methanol sesquisolvate}$

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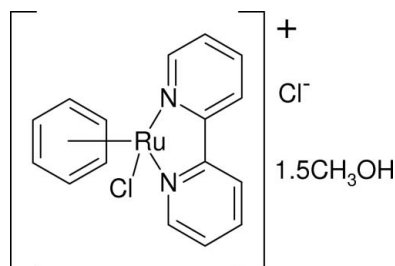
Received 9 November 2007; accepted 13 December 2007

Key indicators: single-crystal X-ray study;  $T = 93\text{ K}$ ; mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$ ; disorder in solvent or counterion;  $R$  factor = 0.033;  $wR$  factor = 0.086; data-to-parameter ratio = 14.0.

In the title compound,  $[\text{RuCl}(\text{C}_6\text{H}_6)(\text{C}_{10}\text{H}_8\text{N}_2)]\text{Cl}\cdot 1.5\text{CH}_3\text{O}$ , the  $\text{Ru}^{\text{II}}$  atom is in a distorted octahedral environment coordinated by an  $\eta^6$ -benzene ring, a chelating 2,2'-bipyridine ligand and a chloride ion. The asymmetric unit is completed by a chloride anion and two methanol molecules, one of which is disordered about a centre of inversion with an occupancy of 0.5. It is an example of a ruthenium complex with a less sterically congested environment than in similar derivatives. In the crystal structure,  $\text{O}-\text{H}\cdots\text{Cl}$  hydrogen bonds, together with  $\pi-\pi$  stacking interactions [centroid-centroid distances of  $3.472\text{ \AA}(2)\text{ \AA}$ ], stabilize the structure.

## Related literature

For literature concerning the synthesis of this class of compound, see Freedman *et al.* (2001). For related structures, see Himeda *et al.* (2007); Lalrempuia & Kollipara (2003).



## Experimental

### Crystal data

$[\text{RuCl}(\text{C}_6\text{H}_6)(\text{C}_{10}\text{H}_8\text{N}_2)]\text{Cl}\cdot 1.5\text{CH}_3\text{O}$   
 $M_r = 454.33$   
 Triclinic,  $P\bar{1}$   
 $a = 6.9027(11)\text{ \AA}$   
 $b = 10.2346(16)\text{ \AA}$

$c = 12.895(2)\text{ \AA}$   
 $\alpha = 85.597(2)^\circ$   
 $\beta = 84.531(2)^\circ$   
 $\gamma = 75.875(2)^\circ$   
 $V = 878.1(2)\text{ \AA}^3$   
 $Z = 2$

Mo  $K\alpha$  radiation  
 $\mu = 1.21\text{ mm}^{-1}$

$T = 93(2)\text{ K}$   
 $0.36 \times 0.34 \times 0.13\text{ mm}$

### Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2007)  
 $T_{\text{min}} = 0.660$ ,  $T_{\text{max}} = 0.854$

4385 measured reflections  
 3082 independent reflections  
 2867 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.014$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.086$   
 $S = 1.06$   
 3082 reflections

220 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.13\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.69\text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ru1—N1	2.083 (3)	Ru1—C2	2.198 (4)
Ru1—N2	2.084 (3)	Ru1—C4	2.198 (4)
Ru1—C1	2.165 (4)	Ru1—C3	2.199 (4)
Ru1—C6	2.186 (4)	Ru1—Cl1	2.4105 (9)
Ru1—C5	2.193 (4)		
N1—Ru1—N2	77.18 (11)	N2—Ru1—Cl1	86.34 (8)
N1—Ru1—Cl1	84.01 (8)		

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O51—H51 $\cdots$ Cl2	0.84	2.18	3.013 (4)	170
O61—H61 $\cdots$ Cl2	0.84	2.15	2.986 (6)	171

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: publCIF (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2425).

## References

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**supplementary materials**

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## ( $\eta^6$ -Benzene)(2,2'-bipyridine- $\kappa^2N,N'$ )chloridoruthenium(II) chloride methanol sesquisolvate

M. I. J. Polson

### Comment

The desire for a ruthenium complex which could be used to synthesize facially coordinated complexes led to the preparation of the starting material (1) (Freedman *et al.* 2001). It is convenient to use, in that the benzene ring can be readily removed in a photolytic reaction leaving ruthenium with three, vacant, facially arranged coordination sites. The Ru<sup>II</sup> atom is in a distorted octahedral environment, Table 1, coordinating to an  $\eta^6$ -benzene ring, a chelating 2,2'-bipyridine ligand and a chloride anion. Compared to other similar complexes from the literature, the cation is less bulky both around the benzene ring (Himeda *et al.*, 2007) and in the bipyridine unit (Lalrempuia & Kollipara, 2003). This manifests itself in two angles. The angles between the mean plane of the bipyridine ligand and the mean plane of the benzene ring (60.47 (18)° in 1) become smaller as the ligands become larger due to additional substitution by methyl groups. This forces the two ligands become more parallel to each other. This effect is seen when either the bipyridine (32.24° Lalrempuia & Kollipara, 2003) or the benzene ring (36.04° Himeda *et al.* 2007) is larger due to additional substitution. With the smaller unsubstituted ligands of (1) the ruthenium atom is also more able to sit in the same plane as the bipyridine ligand, lying only 0.075 (1) Å above the plane in the direction of the chloride ligand. The methanol solvate molecules form O—H...Cl hydrogen bonds to the chloride anion, Table 2, with D—H A distances of 3.013 (4) Å (O51—Cl2) and 2.986 (6) Å (O61—Cl2). The structure is further stabilized by offset  $\pi$ — $\pi$  stacking interactions between adjacent N1, C7...C11 rings of the bipyridine ligands, with centroid to centroid distances of 3.472 (2) Å, related by the symmetry operation 1 - x, 1 - y, 1 - z, Fig. 2.

### Experimental

The complex was prepared according to literature procedures (Freedman *et al.* 2001). X-ray quality crystals were grown by slow evaporation of a solution in methanol.

### Refinement

The C and O atoms of both methanol solvate molecules were refined isotropically. One of these molecules (C60, O60) is disordered about an inversion centre and was refined with the occupancy of all atoms fixed at 0.5. A 11 H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å,  $U_{\text{iso}} = 1.2U_{\text{eq}}$  (C) for aromatic, 0.96 Å,  $U_{\text{iso}} = 1.5U_{\text{eq}}$  (C) for CH<sub>3</sub> atoms and 0.82 Å,  $U_{\text{iso}} = 1.5U_{\text{eq}}$  (O) for the OH groups.

## Figures

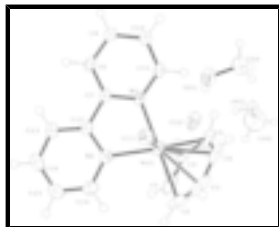


Fig. 1. The molecular structure of (1), showing displacement ellipsoids at the 50% probability level.

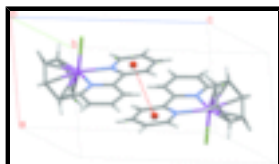


Fig. 2. A packing diagram showing the  $\pi$  stacking. The close centroid-centroid approach is shown as a dashed line.

## $(\eta^6\text{-Benzene})(2,2'\text{-bipyridine-}\kappa^2N,N')$ chloridoruthenium(II) chloride methanol sesquisolvate

### Crystal data

$[\text{RuCl}(\text{C}_6\text{H}_6)(\text{C}_{10}\text{H}_8\text{N}_2)]\text{Cl}\cdot 1.5\text{CH}_4\text{O}$

$M_r = 454.33$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 6.9027(11) \text{ \AA}$

$b = 10.2346(16) \text{ \AA}$

$c = 12.895(2) \text{ \AA}$

$\alpha = 85.597(2)^\circ$

$\beta = 84.531(2)^\circ$

$\gamma = 75.875(2)^\circ$

$V = 878.1(2) \text{ \AA}^3$

$Z = 2$

$F_{000} = 458$

$D_x = 1.718 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3474 reflections

$\theta = 2.5\text{--}26.4^\circ$

$\mu = 1.21 \text{ mm}^{-1}$

$T = 93(2) \text{ K}$

Block, yellow

$0.36 \times 0.34 \times 0.13 \text{ mm}$

### Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 93(2) \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Bruker, 2007)

$T_{\min} = 0.660$ ,  $T_{\max} = 0.854$

4385 measured reflections

3082 independent reflections

2867 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$

$\theta_{\max} = 25.1^\circ$

$\theta_{\min} = 2.5^\circ$

$h = -8 \rightarrow 8$

$k = -12 \rightarrow 12$

$l = -15 \rightarrow 10$

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.086$	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.5007P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3082 reflections	$(\Delta/\sigma)_{\max} < 0.001$
220 parameters	$\Delta\rho_{\max} = 1.13 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.69 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ru1	0.60854 (4)	0.67682 (3)	0.77268 (2)	0.02474 (11)	
Cl1	0.89451 (12)	0.76724 (9)	0.71514 (7)	0.0277 (2)	
Cl2	0.12633 (18)	0.29047 (14)	0.82005 (9)	0.0536 (3)	
N1	0.6736 (4)	0.5821 (3)	0.6319 (2)	0.0217 (6)	
N2	0.4510 (4)	0.8207 (3)	0.6686 (2)	0.0244 (6)	
C7	0.6008 (5)	0.6559 (3)	0.5465 (2)	0.0201 (7)	
C12	0.4677 (5)	0.7878 (3)	0.5677 (3)	0.0217 (7)	
C2	0.4713 (8)	0.7559 (5)	0.9230 (3)	0.0530 (13)	
H2	0.4272	0.8559	0.9289	0.064*	
C1	0.3440 (7)	0.6888 (5)	0.8796 (3)	0.0463 (11)	
H1	0.2101	0.7407	0.8579	0.056*	
C6	0.4177 (8)	0.5533 (5)	0.8541 (3)	0.0499 (13)	
H6	0.3375	0.5085	0.8140	0.060*	
C3	0.6688 (8)	0.6925 (6)	0.9351 (3)	0.0557 (14)	
H3	0.7634	0.7478	0.9496	0.067*	
C4	0.7456 (8)	0.5604 (6)	0.9086 (3)	0.0515 (12)	
H4	0.8939	0.5224	0.9047	0.062*	
C5	0.6250 (8)	0.4896 (5)	0.8699 (3)	0.0489 (12)	

## supplementary materials

H5	0.6880	0.4012	0.8385	0.059*	
C11	0.7918 (5)	0.4575 (3)	0.6204 (3)	0.0234 (7)	
H11	0.8430	0.4054	0.6803	0.028*	
C8	0.6504 (5)	0.6079 (3)	0.4470 (2)	0.0220 (7)	
H8	0.6023	0.6628	0.3876	0.026*	
C9	0.7708 (5)	0.4794 (4)	0.4354 (3)	0.0232 (7)	
H9	0.8048	0.4442	0.3682	0.028*	
C10	0.8406 (5)	0.4030 (4)	0.5234 (3)	0.0236 (7)	
H10	0.9215	0.3140	0.5174	0.028*	
C14	0.2393 (5)	0.9964 (4)	0.5210 (3)	0.0307 (8)	
H14	0.1655	1.0562	0.4708	0.037*	
C13	0.3616 (5)	0.8737 (4)	0.4923 (3)	0.0255 (7)	
H13	0.3729	0.8485	0.4222	0.031*	
C16	0.3322 (5)	0.9412 (4)	0.6948 (3)	0.0307 (8)	
H16	0.3216	0.9650	0.7652	0.037*	
C15	0.2259 (5)	1.0307 (4)	0.6237 (3)	0.0337 (9)	
H15	0.1444	1.1150	0.6447	0.040*	
O51	0.5683 (5)	0.2257 (4)	0.7539 (3)	0.0553 (8)	
H51	0.4459	0.2334	0.7716	0.083*	
C50	0.6807 (7)	0.1122 (5)	0.8067 (4)	0.0484 (11)	
H50A	0.5976	0.0837	0.8658	0.073*	
H50B	0.7973	0.1347	0.8322	0.073*	
H50C	0.7261	0.0388	0.7590	0.073*	
O61	0.1958 (9)	0.0351 (6)	0.9544 (5)	0.0413 (13)*	0.50
H61	0.1872	0.1092	0.9201	0.062*	0.50
C60	-0.002 (4)	0.035 (3)	1.016 (2)	0.135 (8)*	0.50
H60A	0.0149	0.0364	1.0909	0.202*	0.50
H60B	-0.0448	-0.0459	1.0032	0.202*	0.50
H60C	-0.1028	0.1156	0.9950	0.202*	0.50

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ru1	0.02860 (18)	0.03351 (18)	0.01564 (16)	-0.01396 (12)	-0.00330 (11)	-0.00015 (11)
C11	0.0235 (4)	0.0287 (4)	0.0335 (5)	-0.0100 (3)	-0.0057 (3)	-0.0006 (3)
C12	0.0509 (7)	0.0718 (8)	0.0416 (6)	-0.0182 (6)	-0.0168 (5)	0.0028 (5)
N1	0.0215 (14)	0.0283 (15)	0.0187 (13)	-0.0131 (12)	-0.0036 (11)	0.0024 (11)
N2	0.0206 (14)	0.0305 (16)	0.0246 (15)	-0.0109 (12)	-0.0005 (11)	-0.0024 (12)
C7	0.0175 (16)	0.0258 (17)	0.0203 (16)	-0.0120 (13)	-0.0044 (12)	0.0032 (13)
C12	0.0176 (16)	0.0281 (17)	0.0231 (16)	-0.0140 (14)	-0.0012 (13)	0.0022 (13)
C2	0.072 (3)	0.064 (3)	0.028 (2)	-0.031 (3)	0.017 (2)	-0.015 (2)
C1	0.041 (2)	0.076 (3)	0.0229 (19)	-0.021 (2)	0.0037 (17)	0.008 (2)
C6	0.073 (3)	0.081 (3)	0.0145 (18)	-0.058 (3)	-0.0018 (19)	0.0070 (19)
C3	0.065 (3)	0.099 (4)	0.0178 (19)	-0.046 (3)	-0.0041 (19)	-0.006 (2)
C4	0.054 (3)	0.085 (4)	0.0195 (19)	-0.027 (3)	-0.0085 (19)	0.016 (2)
C5	0.074 (3)	0.048 (3)	0.022 (2)	-0.020 (2)	0.007 (2)	0.0148 (18)
C11	0.0226 (17)	0.0259 (17)	0.0242 (17)	-0.0112 (14)	-0.0059 (13)	0.0049 (13)
C8	0.0191 (16)	0.0318 (18)	0.0176 (16)	-0.0122 (14)	-0.0039 (12)	0.0046 (13)

C9	0.0179 (16)	0.0344 (19)	0.0217 (16)	-0.0140 (14)	-0.0014 (13)	-0.0033 (14)
C10	0.0167 (16)	0.0267 (17)	0.0298 (18)	-0.0096 (14)	-0.0039 (13)	0.0007 (14)
C14	0.0183 (17)	0.0299 (19)	0.046 (2)	-0.0122 (15)	-0.0043 (15)	0.0085 (16)
C13	0.0214 (17)	0.0291 (18)	0.0296 (18)	-0.0138 (14)	-0.0050 (14)	0.0045 (14)
C16	0.0263 (19)	0.036 (2)	0.0326 (19)	-0.0139 (16)	0.0049 (15)	-0.0091 (16)
C15	0.0213 (18)	0.0283 (19)	0.051 (2)	-0.0086 (15)	0.0045 (16)	-0.0028 (17)
O51	0.063 (2)	0.058 (2)	0.0437 (18)	-0.0138 (17)	-0.0090 (16)	0.0107 (15)
C50	0.048 (3)	0.042 (2)	0.054 (3)	-0.010 (2)	-0.012 (2)	0.005 (2)

*Geometric parameters (Å, °)*

Ru1—N1	2.083 (3)	C4—H4	1.0000
Ru1—N2	2.084 (3)	C5—H5	1.0000
Ru1—C1	2.165 (4)	C11—C10	1.387 (5)
Ru1—C6	2.186 (4)	C11—H11	0.9500
Ru1—C5	2.193 (4)	C8—C9	1.385 (5)
Ru1—C2	2.198 (4)	C8—H8	0.9500
Ru1—C4	2.198 (4)	C9—C10	1.384 (5)
Ru1—C3	2.199 (4)	C9—H9	0.9500
Ru1—C11	2.4105 (9)	C10—H10	0.9500
N1—C11	1.346 (4)	C14—C15	1.385 (6)
N1—C7	1.352 (4)	C14—C13	1.386 (5)
N2—C16	1.351 (5)	C14—H14	0.9500
N2—C12	1.356 (4)	C13—H13	0.9500
C7—C8	1.392 (5)	C16—C15	1.374 (6)
C7—C12	1.464 (5)	C16—H16	0.9500
C12—C13	1.394 (5)	C15—H15	0.9500
C2—C3	1.378 (8)	O51—C50	1.398 (6)
C2—C1	1.417 (7)	O51—H51	0.8400
C2—H2	1.0000	C50—H50A	0.9800
C1—C6	1.408 (7)	C50—H50B	0.9800
C1—H1	1.0000	C50—H50C	0.9800
C6—C5	1.447 (7)	O61—C60	1.51 (3)
C6—H6	1.0000	O61—H61	0.8400
C3—C4	1.383 (8)	C60—H60A	0.9800
C3—H3	1.0000	C60—H60B	0.9800
C4—C5	1.378 (7)	C60—H60C	0.9800
N1—Ru1—N2	77.18 (11)	C1—C6—Ru1	70.3 (2)
N1—Ru1—C1	127.42 (15)	C5—C6—Ru1	70.9 (2)
N2—Ru1—C1	91.75 (15)	C1—C6—H6	120.4
N1—Ru1—C6	99.21 (14)	C5—C6—H6	120.4
N2—Ru1—C6	111.47 (16)	Ru1—C6—H6	120.4
C1—Ru1—C6	37.76 (19)	C2—C3—C4	120.9 (5)
N1—Ru1—C5	94.95 (14)	C2—C3—Ru1	71.7 (2)
N2—Ru1—C5	148.17 (16)	C4—C3—Ru1	71.6 (2)
C1—Ru1—C5	68.40 (19)	C2—C3—H3	119.0
C6—Ru1—C5	38.58 (19)	C4—C3—H3	119.0
N1—Ru1—C2	165.29 (15)	Ru1—C3—H3	119.0
N2—Ru1—C2	101.06 (17)	C5—C4—C3	120.4 (5)

## supplementary materials

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C1—Ru1—C2	37.89 (18)	C5—C4—Ru1	71.5 (2)
C6—Ru1—C2	67.59 (18)	C3—C4—Ru1	71.7 (3)
C5—Ru1—C2	78.80 (19)	C5—C4—H4	119.3
N1—Ru1—C4	116.02 (17)	C3—C4—H4	119.3
N2—Ru1—C4	166.80 (17)	Ru1—C4—H4	119.3
C1—Ru1—C4	80.20 (18)	C4—C5—C6	120.4 (5)
C6—Ru1—C4	68.00 (18)	C4—C5—Ru1	71.9 (3)
C5—Ru1—C4	36.57 (19)	C6—C5—Ru1	70.5 (2)
C2—Ru1—C4	66.2 (2)	C4—C5—H5	119.1
N1—Ru1—C3	151.14 (18)	C6—C5—H5	119.1
N2—Ru1—C3	130.37 (18)	Ru1—C5—H5	119.1
C1—Ru1—C3	67.60 (18)	N1—C11—C10	121.8 (3)
C6—Ru1—C3	79.73 (17)	N1—C11—H11	119.1
C5—Ru1—C3	66.1 (2)	C10—C11—H11	119.1
C2—Ru1—C3	36.5 (2)	C9—C8—C7	119.3 (3)
C4—Ru1—C3	36.7 (2)	C9—C8—H8	120.4
N1—Ru1—C11	84.01 (8)	C7—C8—H8	120.4
N2—Ru1—C11	86.34 (8)	C10—C9—C8	118.8 (3)
C1—Ru1—C11	147.23 (14)	C10—C9—H9	120.6
C6—Ru1—C11	162.19 (14)	C8—C9—H9	120.6
C5—Ru1—C11	123.93 (14)	C9—C10—C11	119.6 (3)
C2—Ru1—C11	110.55 (13)	C9—C10—H10	120.2
C4—Ru1—C11	94.76 (13)	C11—C10—H10	120.2
C3—Ru1—C11	89.00 (13)	C15—C14—C13	119.2 (3)
C11—N1—C7	119.0 (3)	C15—C14—H14	120.4
C11—N1—Ru1	124.3 (2)	C13—C14—H14	120.4
C7—N1—Ru1	116.5 (2)	C14—C13—C12	119.1 (3)
C16—N2—C12	118.5 (3)	C14—C13—H13	120.4
C16—N2—Ru1	125.0 (2)	C12—C13—H13	120.4
C12—N2—Ru1	116.5 (2)	N2—C16—C15	122.7 (3)
N1—C7—C8	121.6 (3)	N2—C16—H16	118.6
N1—C7—C12	114.8 (3)	C15—C16—H16	118.6
C8—C7—C12	123.6 (3)	C16—C15—C14	119.0 (3)
N2—C12—C13	121.4 (3)	C16—C15—H15	120.5
N2—C12—C7	114.6 (3)	C14—C15—H15	120.5
C13—C12—C7	124.0 (3)	C50—O51—H51	109.5
C3—C2—C1	120.7 (5)	O51—C50—H50A	109.5
C3—C2—Ru1	71.8 (3)	O51—C50—H50B	109.5
C1—C2—Ru1	69.8 (2)	H50A—C50—H50B	109.5
C3—C2—H2	118.9	O51—C50—H50C	109.5
C1—C2—H2	118.9	H50A—C50—H50C	109.5
Ru1—C2—H2	118.9	H50B—C50—H50C	109.5
C6—C1—C2	119.4 (5)	C60—O61—H61	109.5
C6—C1—Ru1	71.9 (2)	O61—C60—H60A	109.5
C2—C1—Ru1	72.3 (2)	O61—C60—H60B	109.5
C6—C1—H1	120.0	H60A—C60—H60B	109.5
C2—C1—H1	120.0	O61—C60—H60C	109.5
Ru1—C1—H1	120.0	H60A—C60—H60C	109.5
C1—C6—C5	118.2 (4)	H60B—C60—H60C	109.5

*Hydrogen-bond geometry (Å, °)*

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
O51—H51···Cl2	0.84	2.18	3.013 (4)	170
O61—H61···Cl2	0.84	2.15	2.986 (6)	171

Fig. 1

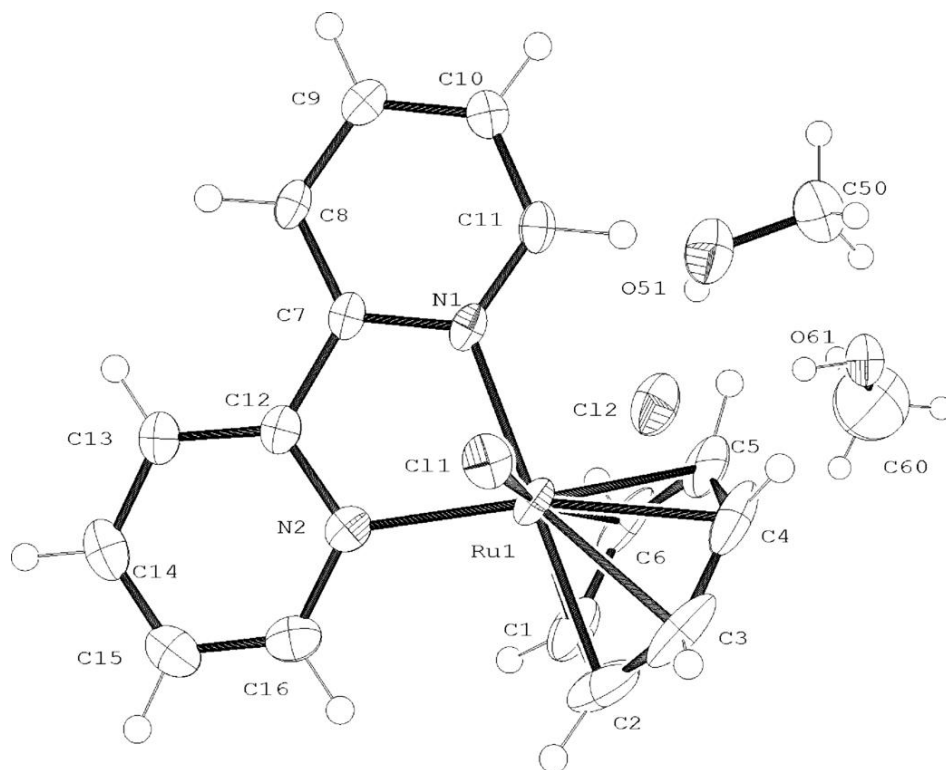


Fig. 2

