Supporting Information Part 1

Synthesis and characterization of new ruthenium *N*-heterocyclic carbene Hoveyda II-type complexes. Study of reactivity in ring closing metathesis reaction

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General procedures

All the reactions were carried out under nitrogen atmosphere. Glassware was dried in an oven at 110 ºC before use. 1,3-Bis(2,4,6-trimethylphenyl)imidazolium chloride was purchased from Strem. The Hoveyda-Grubbs first- and second- generation catalysts were purchased from Aldrich. The solvents were purified by passage through a neutral alumina column under nitrogen. CD_2Cl_2 was distilled from CaH_2 into a Schlenk tube and freeze/pump/thawed 3 times. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with F-254 indicator, visualised by irradiation with UV light. Column chromatography was performed using silica gel Merck 60 (particle size 0.040-0.063 mm). ^{1}H-NMR and ^{13}C-NMR were recorded on a Bruker AV 300 spectrometer in $CDCl_3$. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated s

(singlet), bs (broad singlet), d (doublet), t (triplet), sept (septuplet), m (multiplet); coupling constants (*J*) are in Hertz (Hz).

Stock Solution Preparation

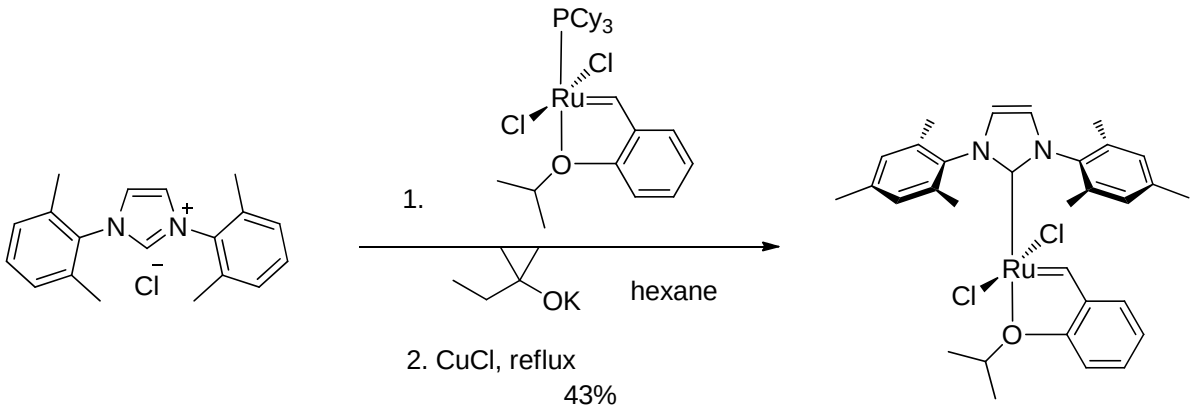
Inside a glovebox, a flask is charged with catalyst (0.016 mmol) and CD_2Cl_2 added to prepare 1.0 mL of stock solution (0.016 M).

RCM of Diethyldiallyl malonate

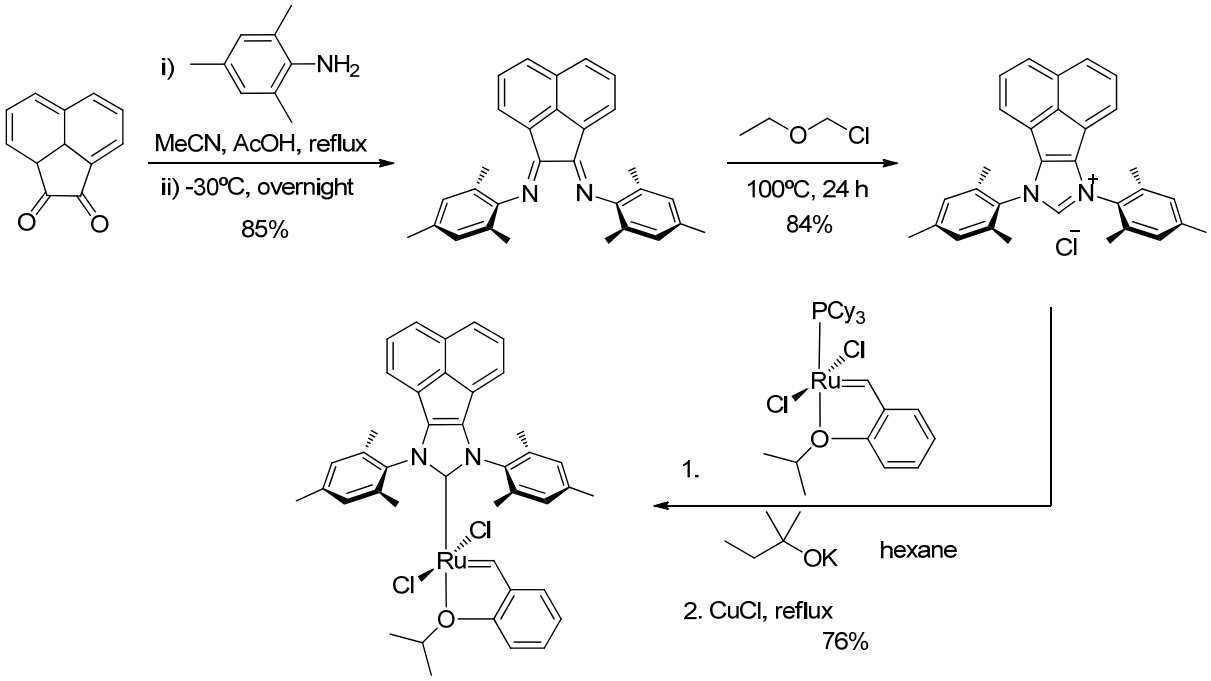
An NMR tube with a screw-cap septum top was charged inside a glovebox with catalyst stock solution (0.016 M, 50 μL, 0.80 μmol, 1.0 mol%) and CD_2Cl_2 (0.75 mL). The sample was equilibrated at 30ºC in the NMR probe before diethyldiallyl malonate (19.3 μL, 19.2 mg, 0.080 mmol, 0.1 M) was added via syringe. The conversion to dimethyl 3-cyclopentene-1,1-dicarboxylate was determined by comparing the ratio of the integrals of the methylene protons in the starting material, δ 2.64 (dt), with those in the product, δ 3.02 (s).

RCM of *N,N´*-diallyl-4-methylbenzenesulfonamide

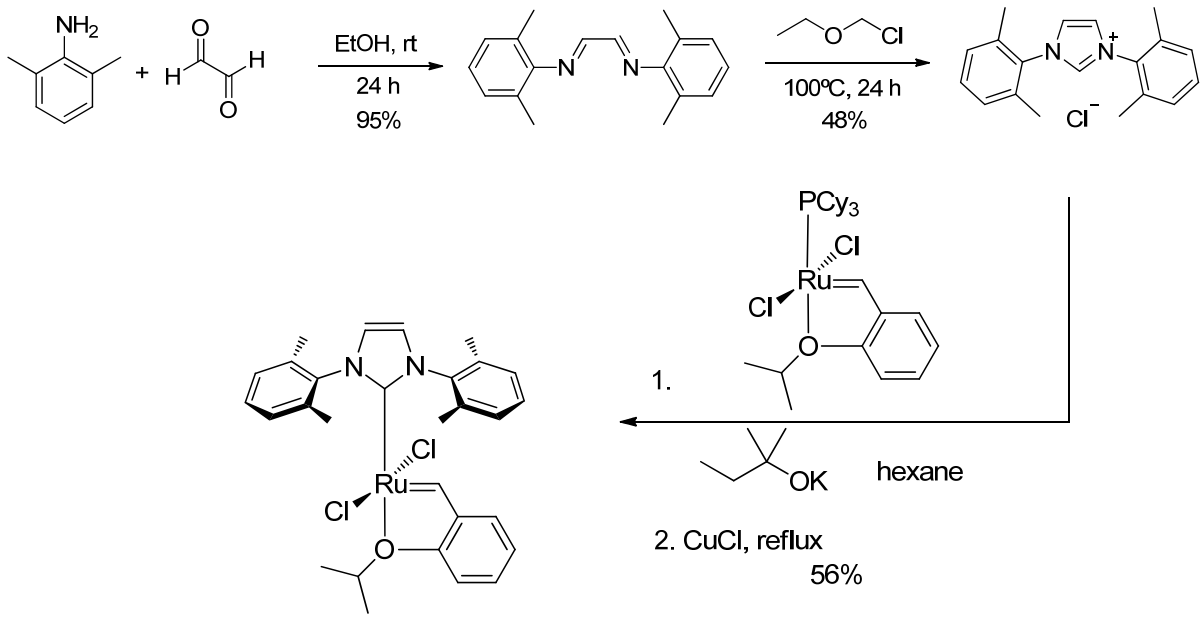
An NMR tube with a screw-cap septum top was charged inside a glovebox with catalyst stock solution (0.016 M, 50 μL, 0.80 μmol, 1.0 mol%) and CD_2Cl_2 (0.75 mL). The sample was equilibrated at 30ºC in the NMR probe before *N,N´*-diallyl-4-methylbenzenesulfonamide (20.1 mg, 0.080 mmol, 0.1 M) was added via syringe. The conversion to 1-tosyl-2,5-dihydro-1H-pyrrole was determined by comparing the ratio of the integrals of the methylene protons in the starting material, δ 3.82 (dt), with those in the product, δ 4.12 (s).



Scheme 1. Synthesis of complex **2**.



Scheme 2. Synthetic route of the complex **3**.



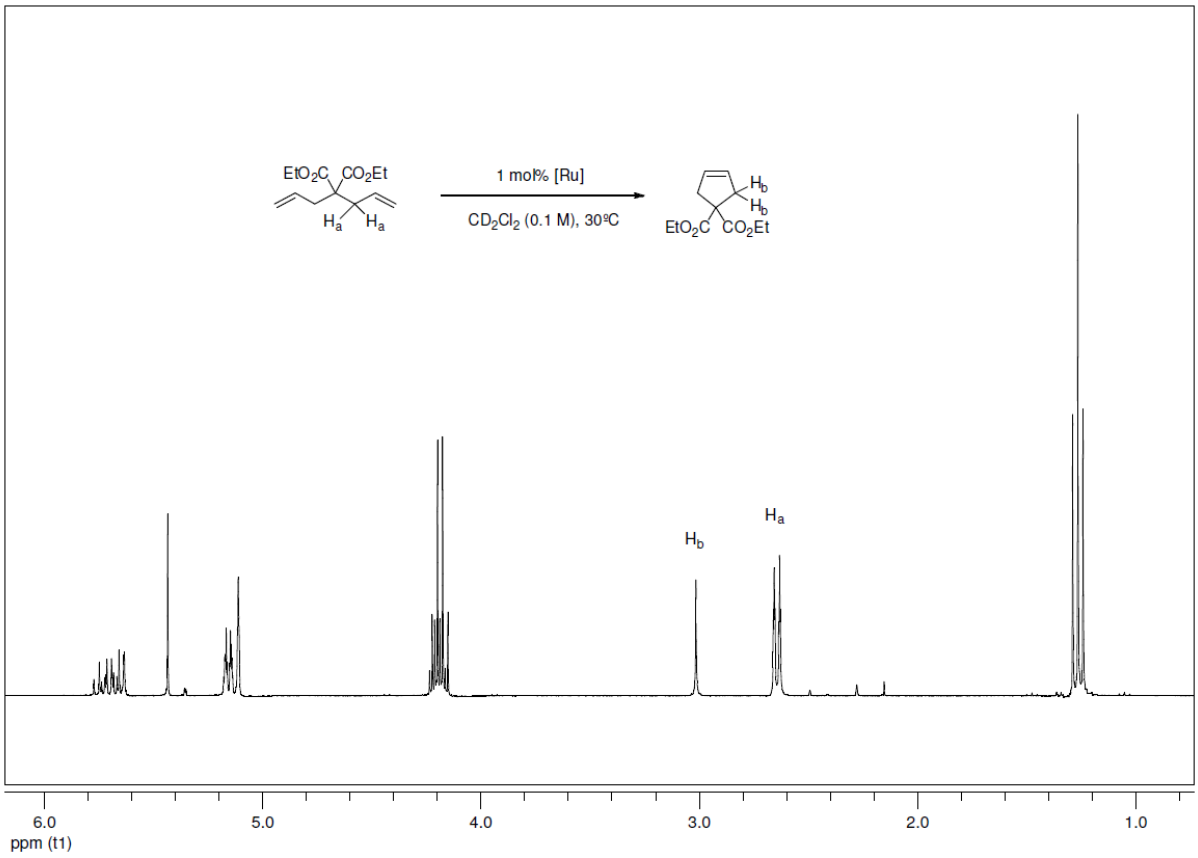
Scheme 3. Synthetic route of the complex **4**.

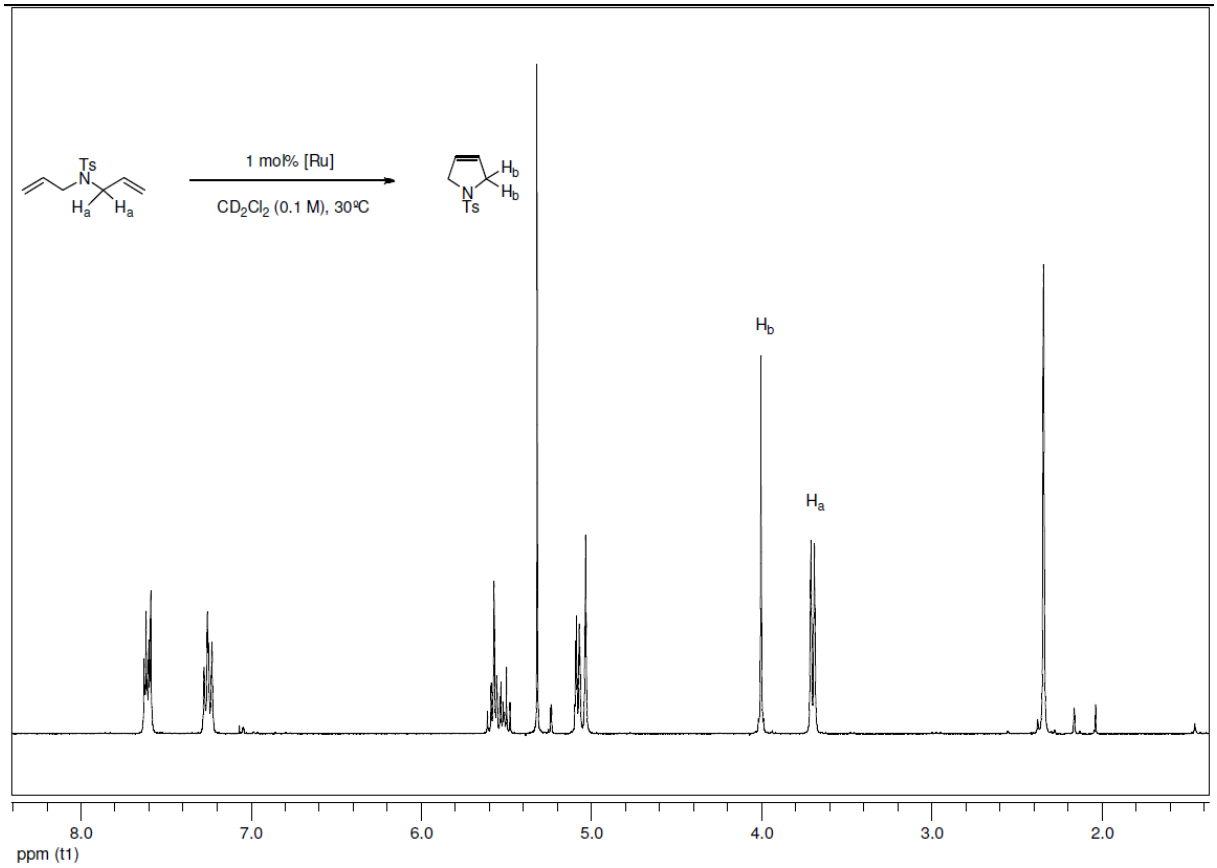
Electrochemical Experiments.

Cyclic voltammetric experiments were performed on an Epsilon Electrochemical Analyzer. A three-electrode cell was used which was equipped with platinum as working electrode, a platinum wire as a counter electrode, and an Ag/AgCl electrode as reference.

Electrochemical measurements were performed at room temperature, under nitrogen atmosphere at 100 $mV \cdot s^{-1}$ in a solution of ruthenium complex in dry dichloromethane (10^{-3} M) containing tetra *n*-butylammonium hexafluorophosphate as the supporting electrolyte.

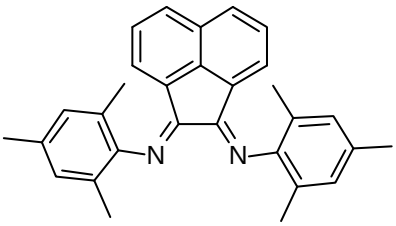
^{1}H NMR Spectra of the reaction mixtures





Physical data

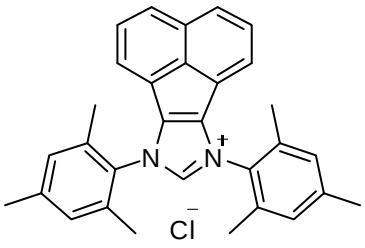
Bis-[*N,N´*-(2,4,6-trimethylphenyl)imino]-acenaphthene[1,2]



Acenaphthenequinone (15.0 g, 82 mmol) was suspended in acetonitrile (500 mL) and heated to 80ºC for 1 hour. Acetic acid (156 mL) was added, and heating was continued until the acenaphthenequinone had completely dissolved. To this hot solution was added 2,4,6-trimethylaniline (25 g, 181 mmol) slowly with a dropping funnel over 20 min. The resulting solution was heated under reflux for another 3 h and cooled to room temperature. After one night at -30ºC, the precipitated orange solid was filtered, washed with pentane and dried in air (28.6 g, 85% yield).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.89 (d, *J* = 8.3 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 2H), 6.98 (s, 4H), 6.77 (d, *J* = 7.2 Hz, 2H), 2.38 (s, 6H), 2.10 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 161.03, 146.74, 140.50, 132.76, 130.96, 129.67, 128.89, 128.73, 128.18, 124.55, 122.44, 20.90, 17.68.

Mes(BIAN) imidazolium chloride[3]



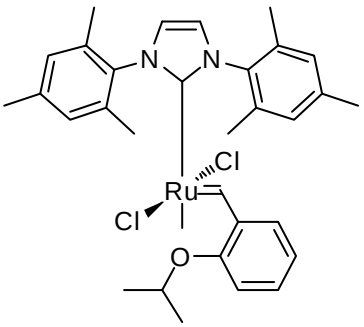
The compound Mes(BIAN) imidazolium chloride was prepared using the method published by Vasudevan *et al.*[4] Mes(BIAN) (1.00 g, 2,4 mmol) and ethoxy(methyl)chloride (4.5 mL, 48 mmol) were added to a Schlenk under nitrogen atmosphere. The reaction mixture was stirred at 100ºC for 24 h. The reaction mixture is cooled at room temperature. Addition of 10 mL of diethyl ether, the resulting yellow solid was filtered, washed with diethyl ether and dried *in vacuo* to afford the product (935 mg, 84% yield).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 10.73 (bs, 1H), 7.99 (d, *J* = 8.3 Hz, 2H), 7.57 (dd, *J* = 8.2 and 7.1 Hz, 2H), 7.29 (d, *J* = 7.0 Hz, 2H), 7.14 (s, 4H), 2.41 (s, 6H), 2.29 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.39, 136.59, 134.02, 130.43, 130.23, 130.17, 129.77, 129.56, 128.14, 123.21, 122.85, 21.22, 17.79; HRMS (ESI): m/z: calcd for $C_{31}H_{29}N_2^+$ *m/z* 429.2325; found: 429.2337.

General procedure to synthesize the ruthenium complexes

The complexes of ruthenium were prepared using the method published by Bieniek et al.[5] A dry Schlenk with a magnetic stirring bar was charged under a nitrogen atmosphere with the corresponding imidazolium salt (0.2 mmol) and dry *n*-hexane (2.4 mL). A solution of potassium *tert*-amylate in toluene (1.7 M solution in toluene, 122 μL, 0.21 mmol) was added to a well-stirred suspension, and the resulting mixture was stirred under nitrogen at room temperature for 1 h. To the resulting solution was added the solid Hoveyda-Grubbs first-generation catalyst (100 mg, 0.17 mmol) in one portion. The Schlenk was equipped with a reflux condenser and the reaction mixture was refluxed for 2 h. After this time, the Schlenk is cooled at room temperature, and CuCl (0.29 mmol) was added in one portion. The resulting mixture was refluxed for 2 h. From this point, all manipulations were carried out in air. The reaction mixture was evaporated to dryness, and the resulting solid was redissolved in ethyl acetate. The solution was filtrated through a Büchner funnel with a glass frit filled with Celite and then concentrated in vacuo. The ruthenium complex was purified by precipitation or column chromatography.

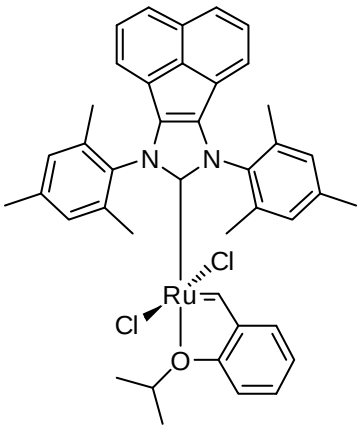
1,3-bis(2,4,6-trimethylphenyl)-2,3-dihydro-1H-imidazole $Cl_2Ru(=CH\text{-}o\text{-}O\text{-}i\text{-}PrC_6H_4)$ (2)



This ruthenium complex was prepared using the general method described previously. The pure product (45.3 mg, 43% yield) was obtained by purification by column chromatography (hexane/ethyl acetate).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 16.71 (s, 1H), 7.49 (ddd, *J* = 8.4, 7.4 and 1.7 Hz, 1H), 7.29-7.26 (m, 1H), 7.12 (m, 5H), 7.01 (dd, *J* = 7.5 and 1.6 Hz, 1H), 6.88 (td, *J* = 7.5 and 0.6 Hz, 1H), 6.83-6.77 (m, 1H), 4.93 (sept, *J* = 6.1 Hz, 1H), 2.45 (s, 6H), 2.27 (s, 12H), 1.36 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 293.3, 175.9, 152.4, 145.5, 139.5, 138.1, 135.9, 129.5, 129.0, 124.7, 122.4, 122.2, 112.9, 75.1, 21.2, 19.0. HRMS (ESI): *m/z* (%): cald for $C_{31}H_{36}Cl_2N_2ORuNa$: 647.1146; found: 647.1127 [M^++Na]; IR (KBr) = 3410, 2920, 1620, 1480, 1310, 1110, 932, 751.

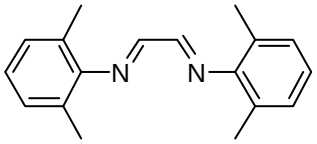
$Cl_2Ru(=CH\text{-}o\text{-}O\text{-}i\text{-}PrC_6H_4)$Mes(BIAN) (3)



The complex with Mes(BIAN) was prepared using the general method described previously. The dark brown residue was dissolved in a 1:10 v/v mixture of CH_2Cl_2 and methanol at room temperature. After concentration of this solution to ca. one-fourth of the initial volume using the rotary evaporator red crystals were precipitated. These crystals were filtered off on a Büchner funnel. The red crystals were washed twice with MeOH and dried in vacuo to give pure catalyst of ruthenium (94.3 mg, 76% yield).

^{1}H NMR (300 MHz, $CDCl_3$): δ = 16.85 (s, 1H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.51 (ddd, *J* = 8.4, 7.5 and 1.7 Hz, 1H), 7.38 (d, *J* = 8.3 Hz, 1H), 7.36 (d, *J* = 8.3 Hz, 1H), 7.20 (s, 4H), 7.05 (dd, *J* = 7.5 and 1.5 Hz, 1H), 6.96 - 6.84 (m, 4H), 4.98 (sept, *J* = 6.1 Hz, 1H), 2.51 (s, 6H), 2.37 (s, 12H), 1.41 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 293.22, 183.93, 152.50, 145.47, 139.71, 139.31, 137.86, 134.54, 129.52, 129.34, 129.23, 127.52, 127.48, 126.03, 122.46, 119.95, 113.03, 75.25, 21.35, 21.21, 19.19; IR (KBr) = 3410, 2920, 1740, 1610, 1490, 1240, 1110, 931, 753.

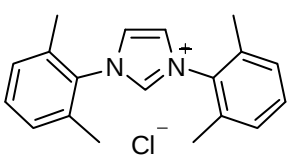
Bis-(2,6-dimethylphenyl)-diazabutadiene



The compound bisimine was prepared using the method published by Türkmen *et al*.[6] To a solution of 2,6-dimethylaniline (3.4 mL, 27.57 mmol) in 275 mL of ethanol was added at 25ºC a mixture of a 40% aqueous solution of glyoxal (1.6 mL, 34.46 mmol). The mixture was stirred for 24 h at room temperature. The resulting yellow solution was concentrated using rotary evaporator and the yellow precipitate was collected by filtration and dried in vacuum (3.46 g, 95% yield). The ^{1}H and ^{13}C NMR spectra were consistent with the reported data.[7]

^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.12 (s, 2H), 7.10 (d, *J* = 7.0 Hz, 4H), 7.01 (d, *J* = 8.5 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 2.19 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 163.45, 149.85, 128.28, 126.42, 124.77, 18.22.

1,3-Bis-(2,6-dimethylphenyl)-1H-imidazol-3-ium trifluoromethanesulfonate

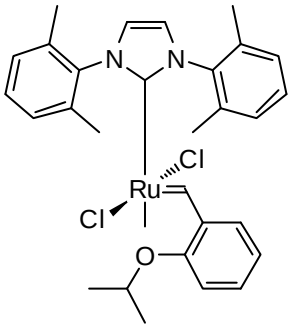


Bis-(2,6-dimethylphenyl)-diazabutadiene (1.00 g, 3,78 mmol) and ethoxy(methyl)chloride (7.0 mL, 75.65 mmol) were added to a Schlenk under nitrogen atmosphere. The reaction mixture was stirred at 100ºC for 24 h. The reaction mixture is cooled at room temperature. The homogeneous solution was concentrated and the residue was dissolved in MeOH. The pure compound was

obtained by precipitation with diethyl ether, filtration and drying under vacuum (567 mg, 48% yield). The ^{1}H and ^{13}C NMR spectra were consistent with the reported data.[8]

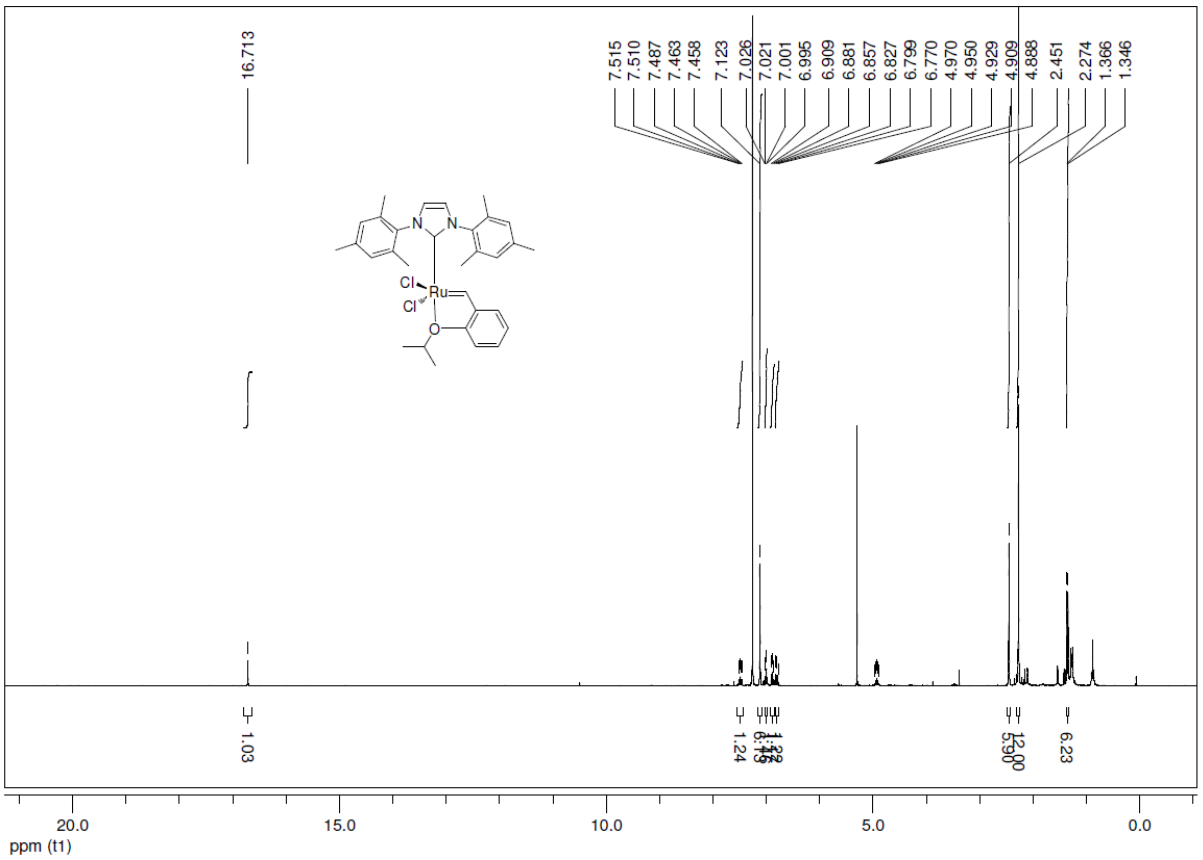
^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.37 (s, 1H), 7.60 (d, *J* = 1.4 Hz, 2H), 7.39 (d, *J* = 7.3 Hz, 1H), 7.37 (d, *J* = 7.3 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 4H), 2.16 (s, 12H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 137.91, 134.39, 132.83, 131.22, 129.25, 124.82, 17.31.

1,3-bis(2,6-dimethylphenyl)-2,3-dihydro-1H-imidazole $Cl_2Ru(=CH\text{-}o\text{-}O\text{-}i\text{-}PrC_6H_4)$ (4)



This ruthenium complex was prepared using the general method described previously. The pure product (55.8 mg, 56% yield) was obtained by purification by column chromatography (hexane/ethyl acetate).

^{1}H NMR (300 MHz, CD_2Cl_2): δ = 16.52 (s, 1H), 7.60 (ddd, *J* = 8.4, 7.4 and 1.7 Hz, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.50 (d, *J* = 8.1 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 4H), 7.24 (s, 2H), 7.11 (dd, *J* = 7.6 and 1.6 Hz, 1H), 6.97 (td, *J* = 7.4 and 0.7 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 4.96 (sept, *J* = 6.2 Hz, 1H), 2.35 (s, 12H), 1.36 (d, *J* = 6.2 Hz, 6H); ^{13}C NMR (75 MHz, CD_2Cl_2): δ = 289.0, 174.9, 152.3, 145.3, 138.4, 129.7, 129.1, 128.5, 125.0, 122.6, 121.9, 113.1, 75.4, 21.1, 19.0; HRMS (ESI): *m/z* (%): cald for $C_{29}H_{32}N_2ORuNa$: 549.1456; found: 549.1497 [M^+-Cl_2+Na]; IR (KBr) = 3410, 2920, 1620, 1480, 1310, 1110, 936, 749.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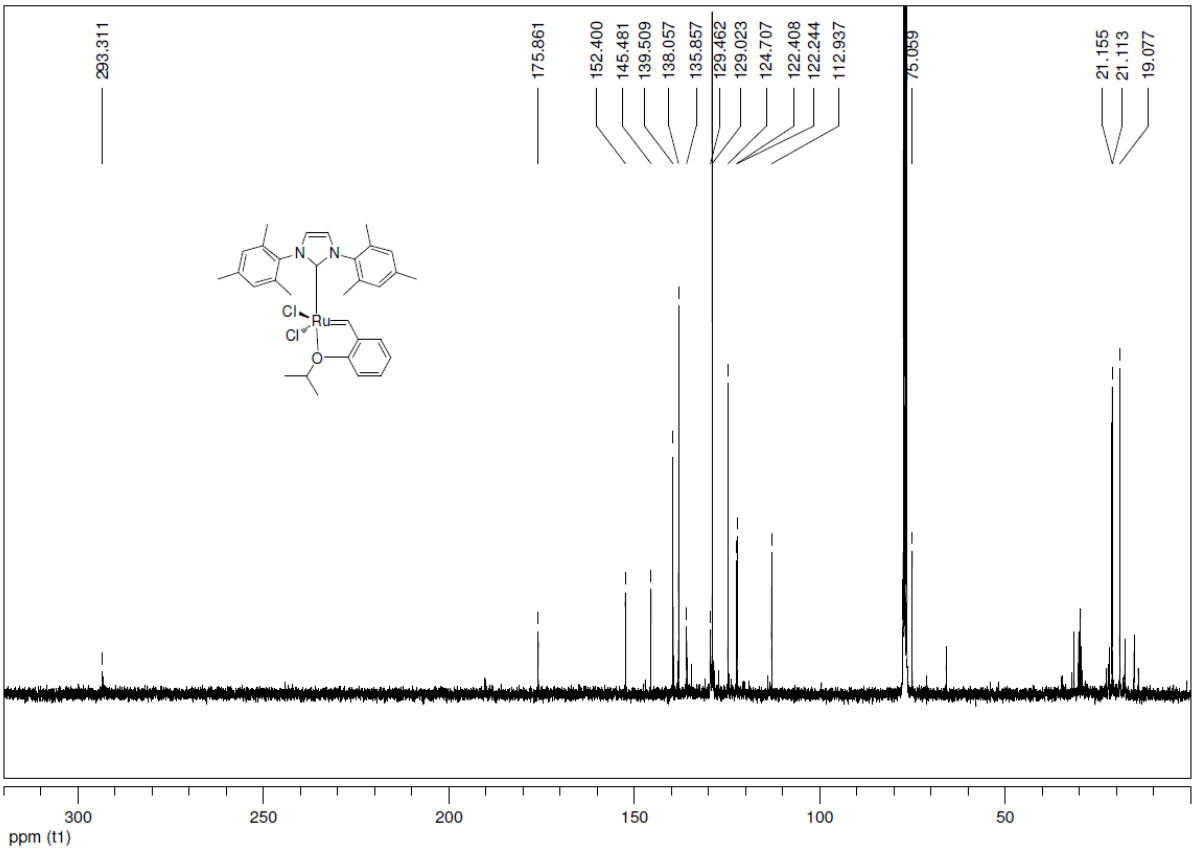
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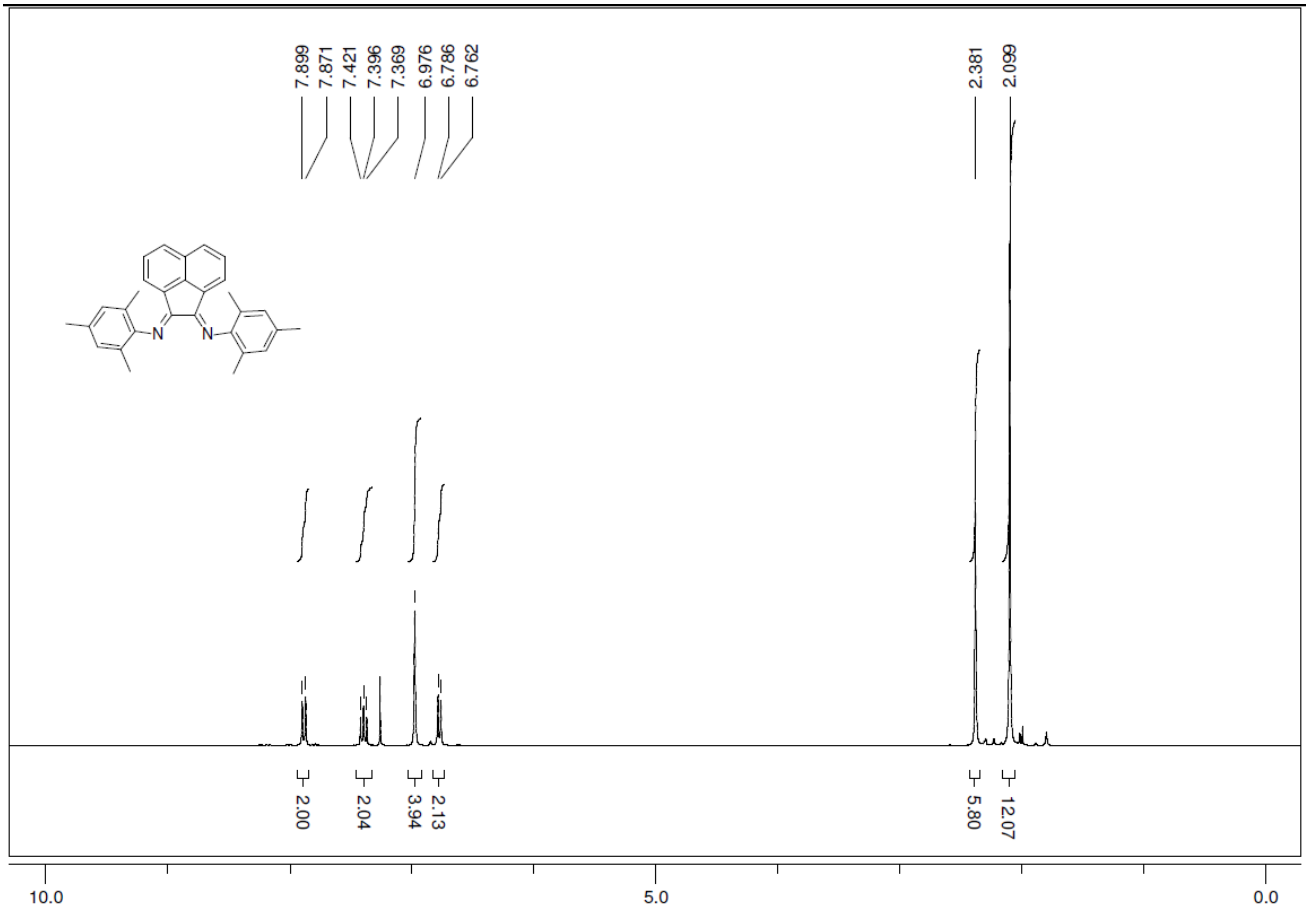
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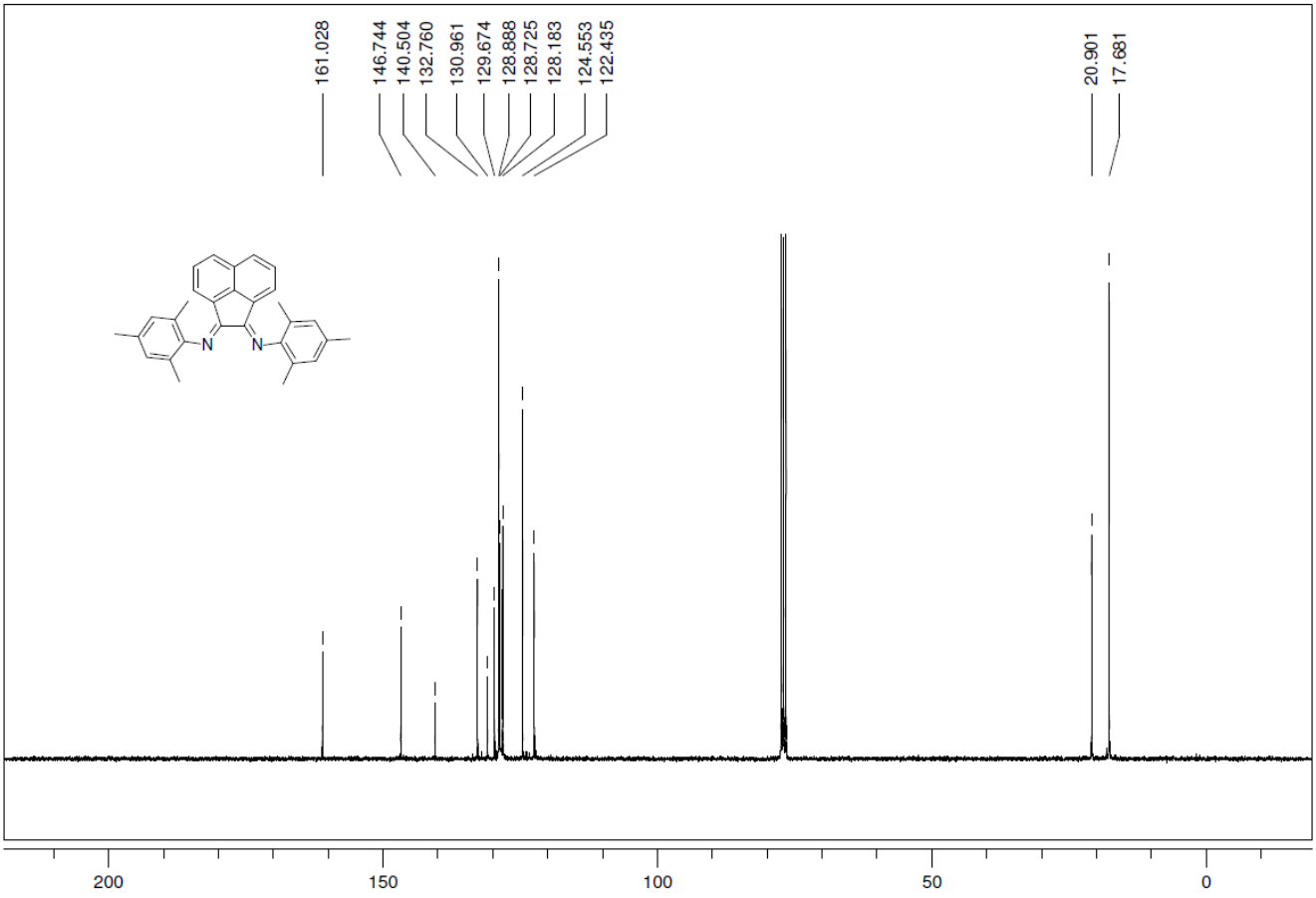
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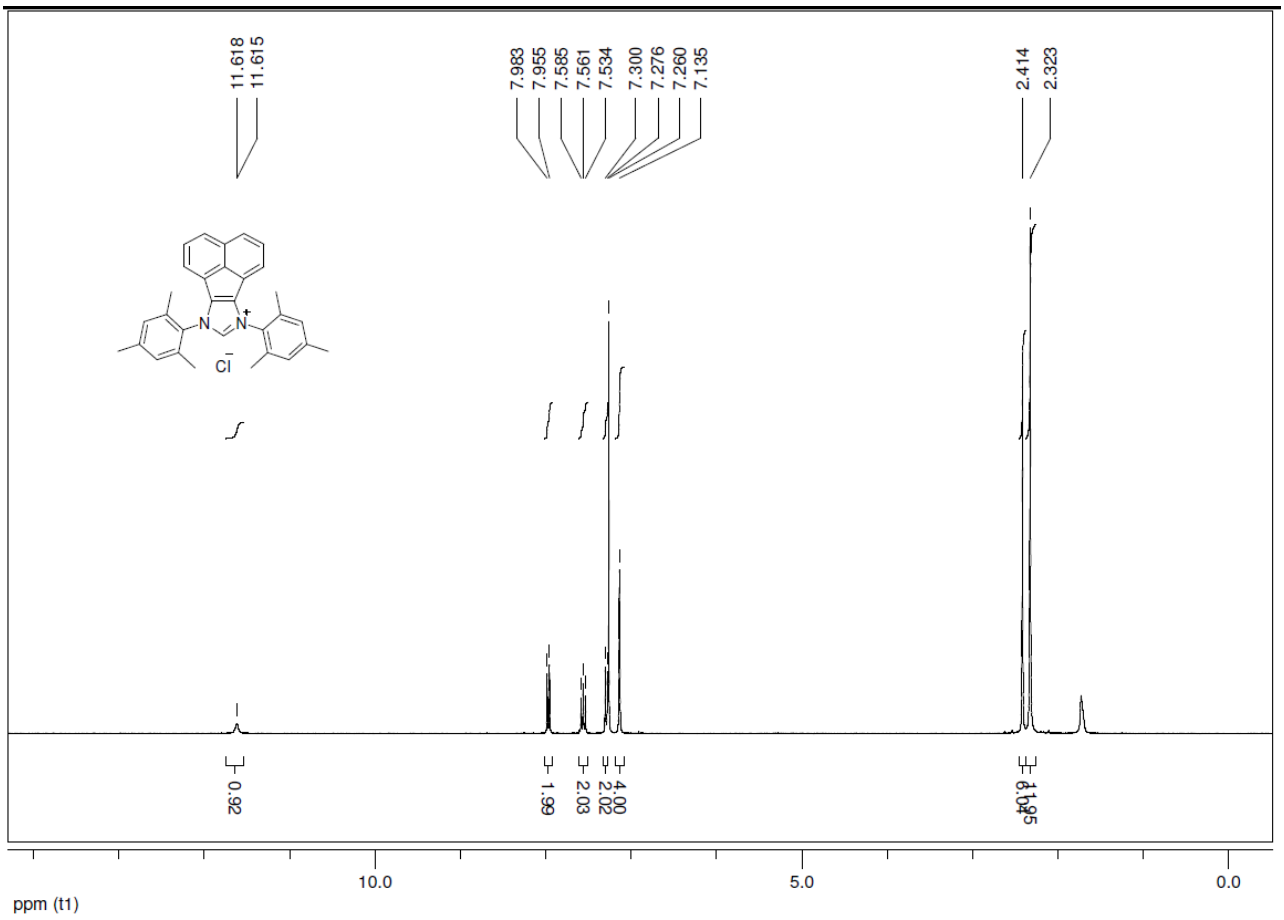
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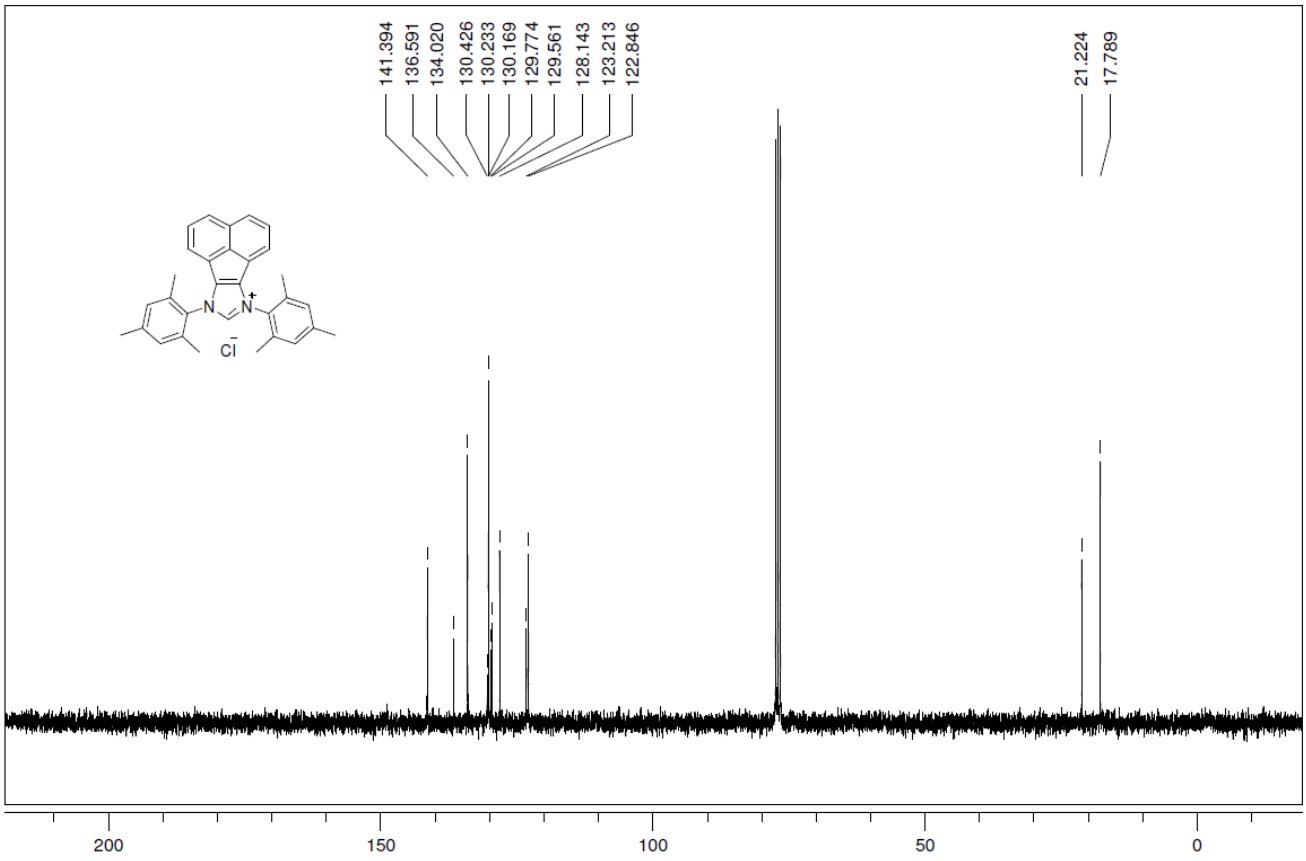
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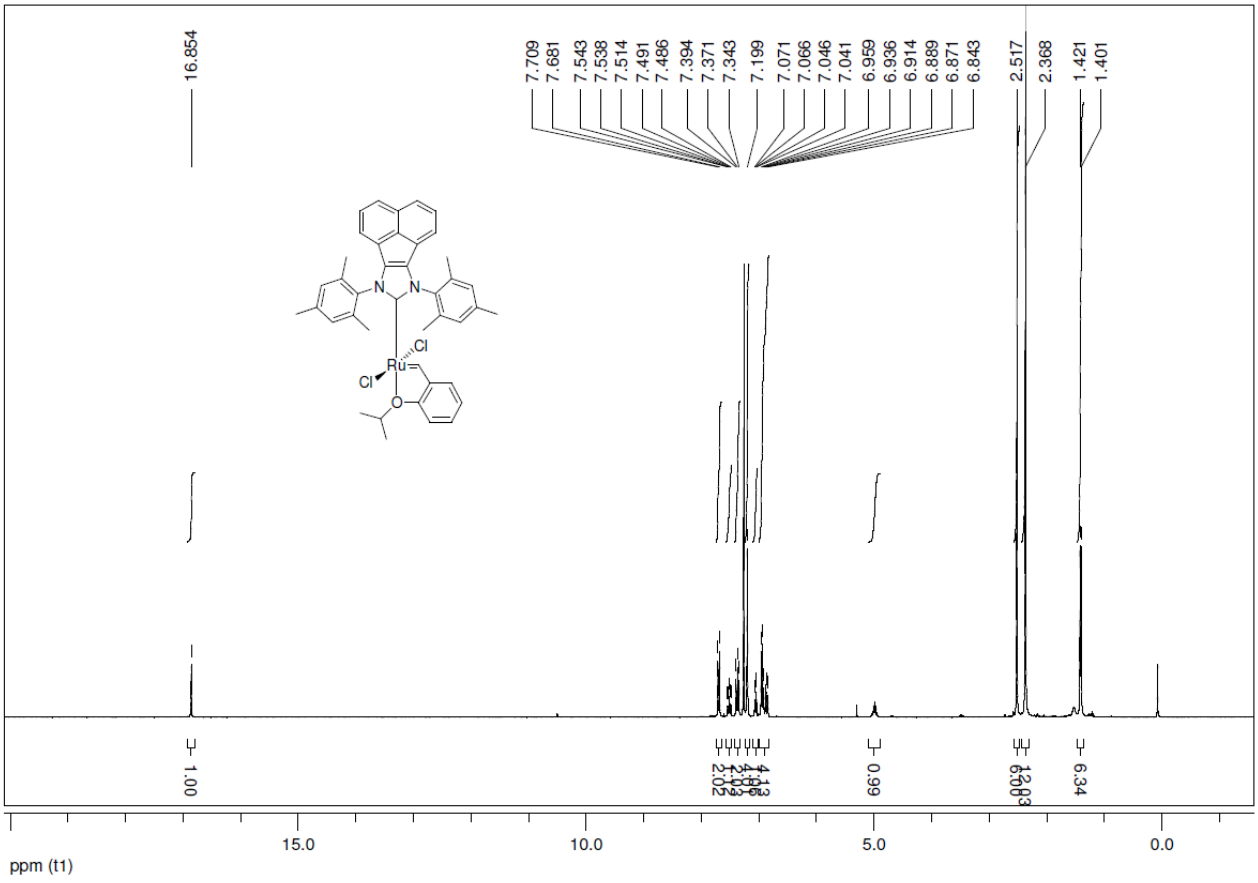

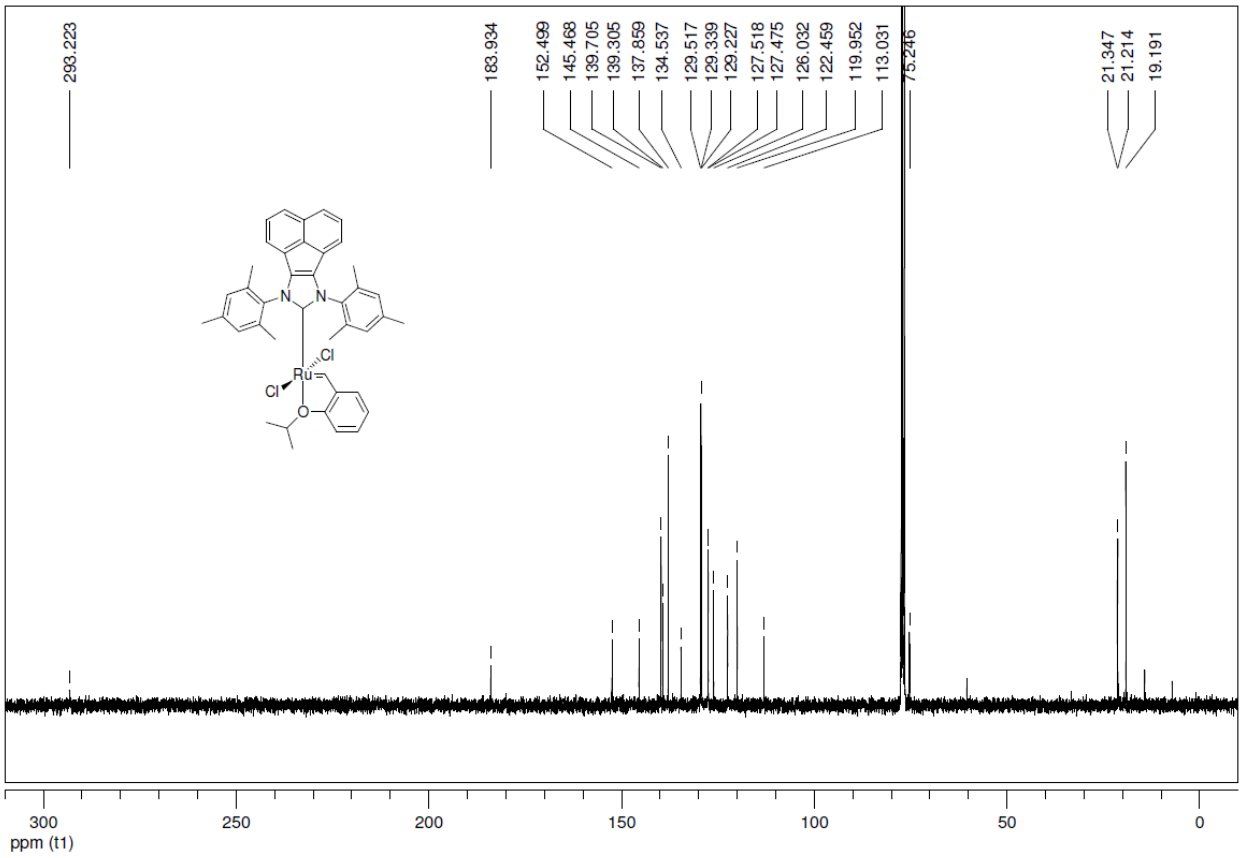

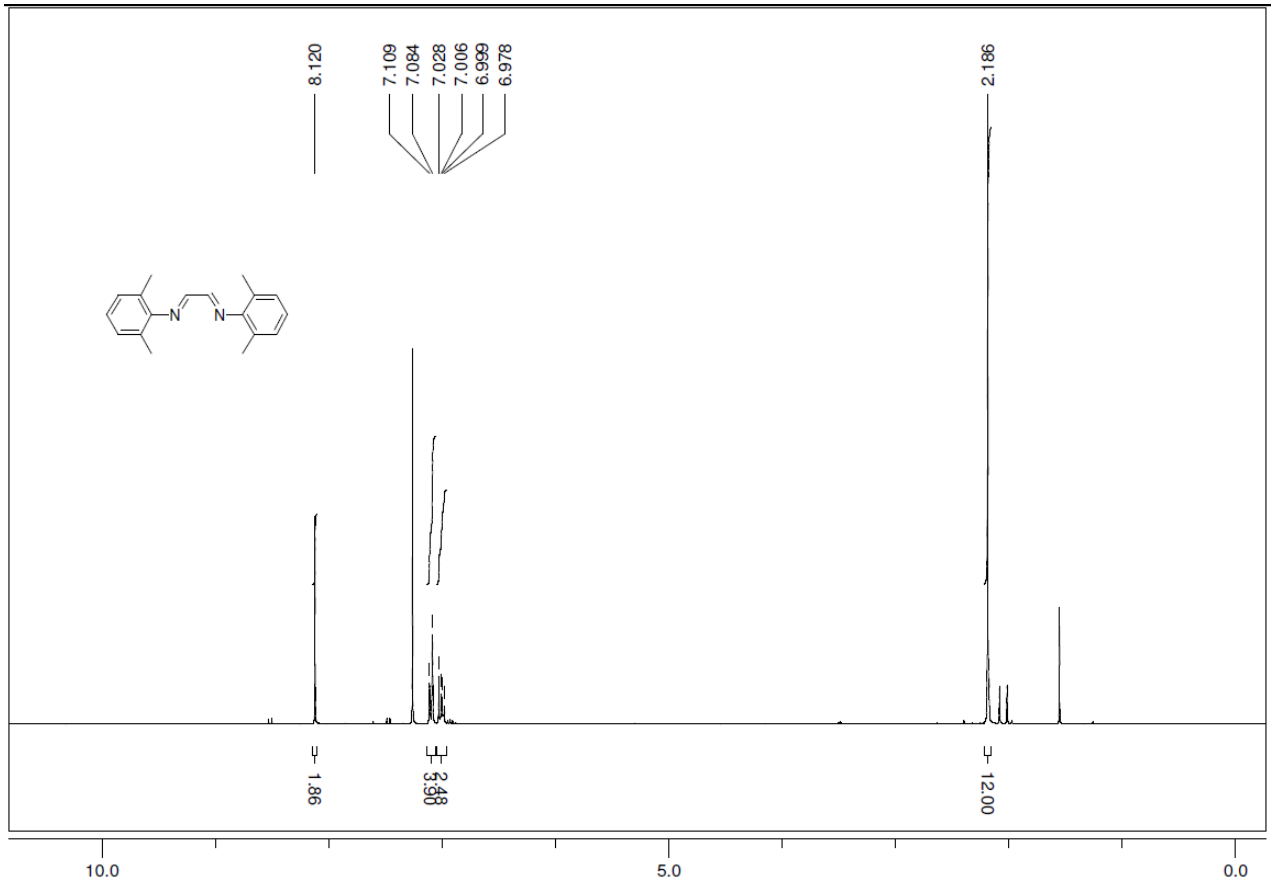

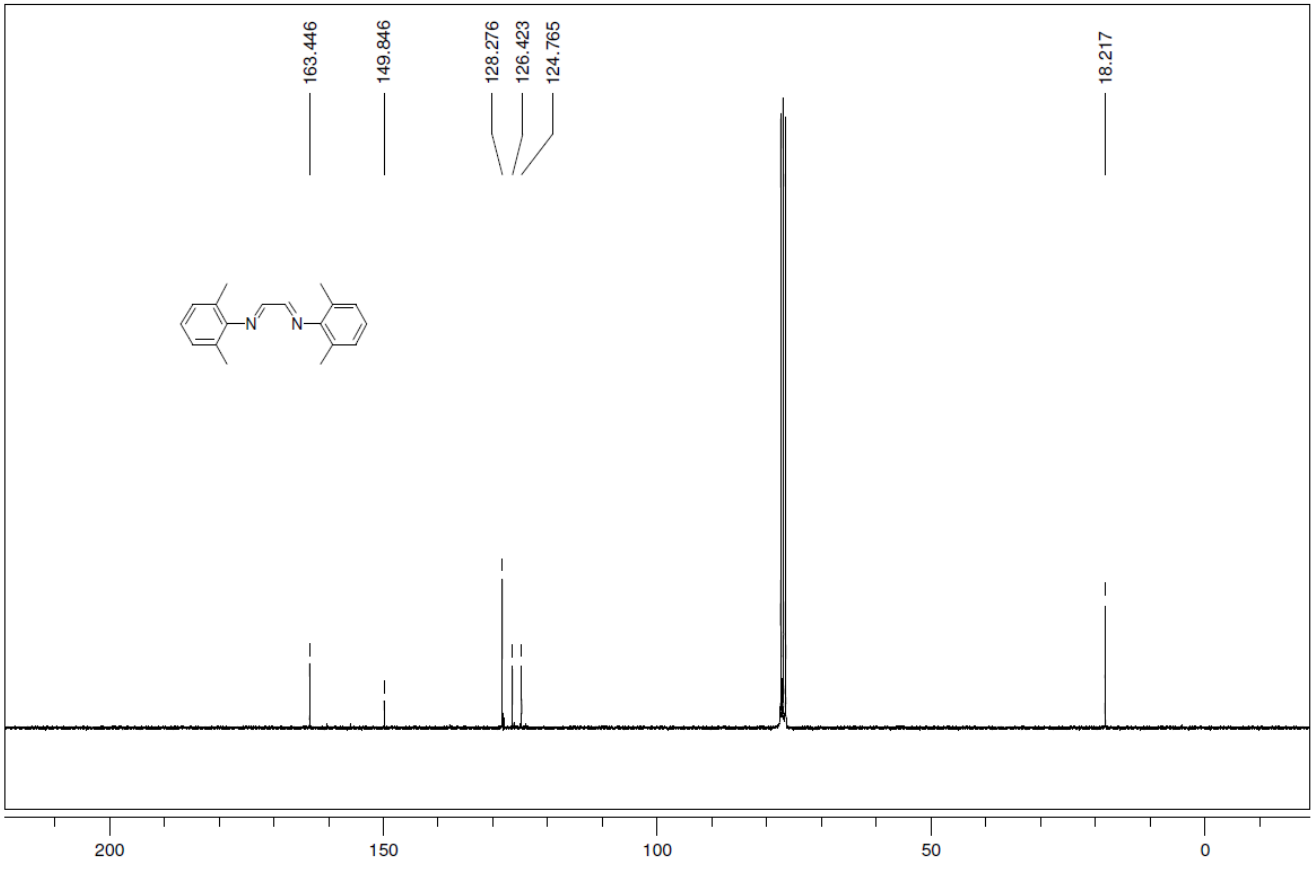

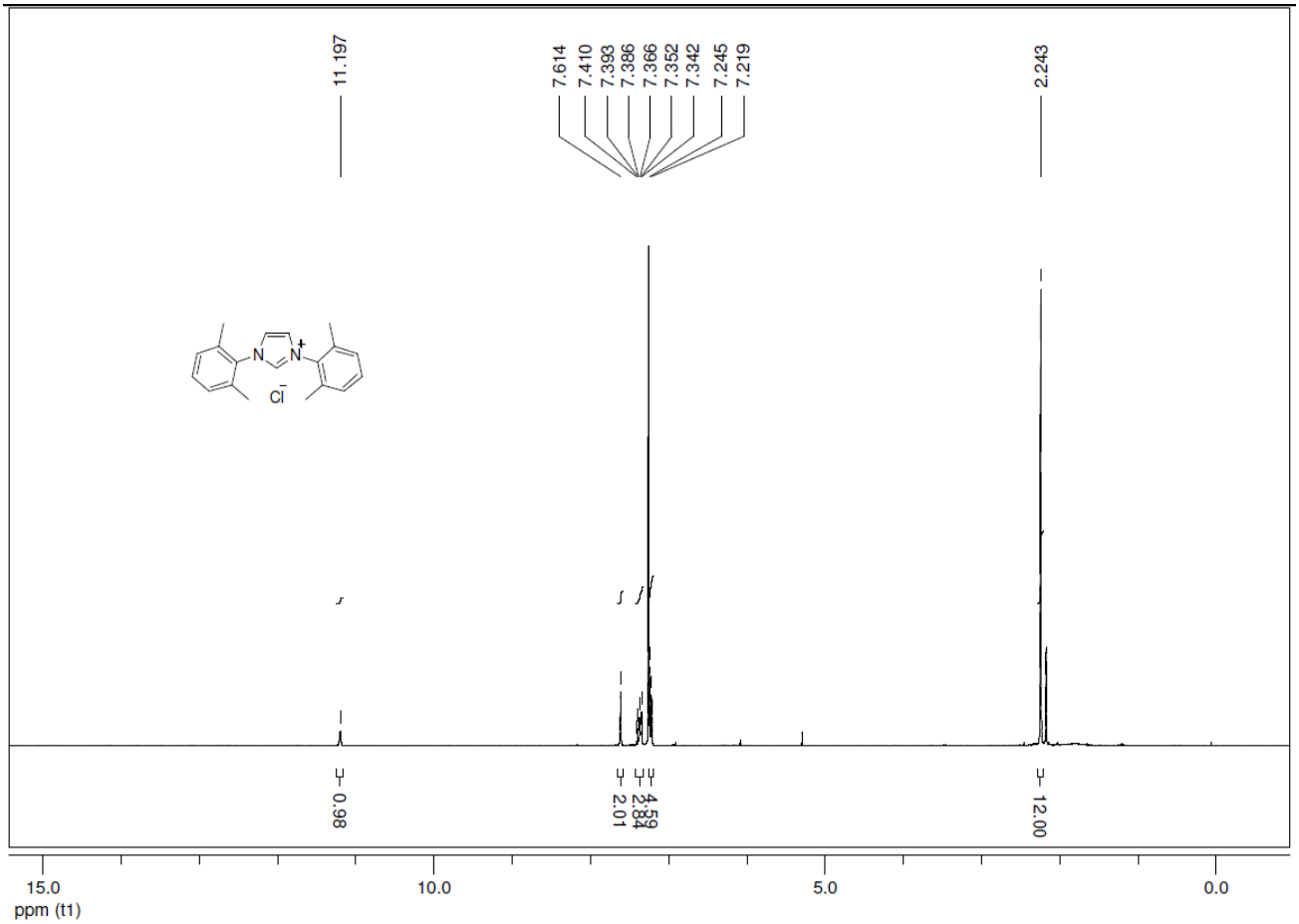

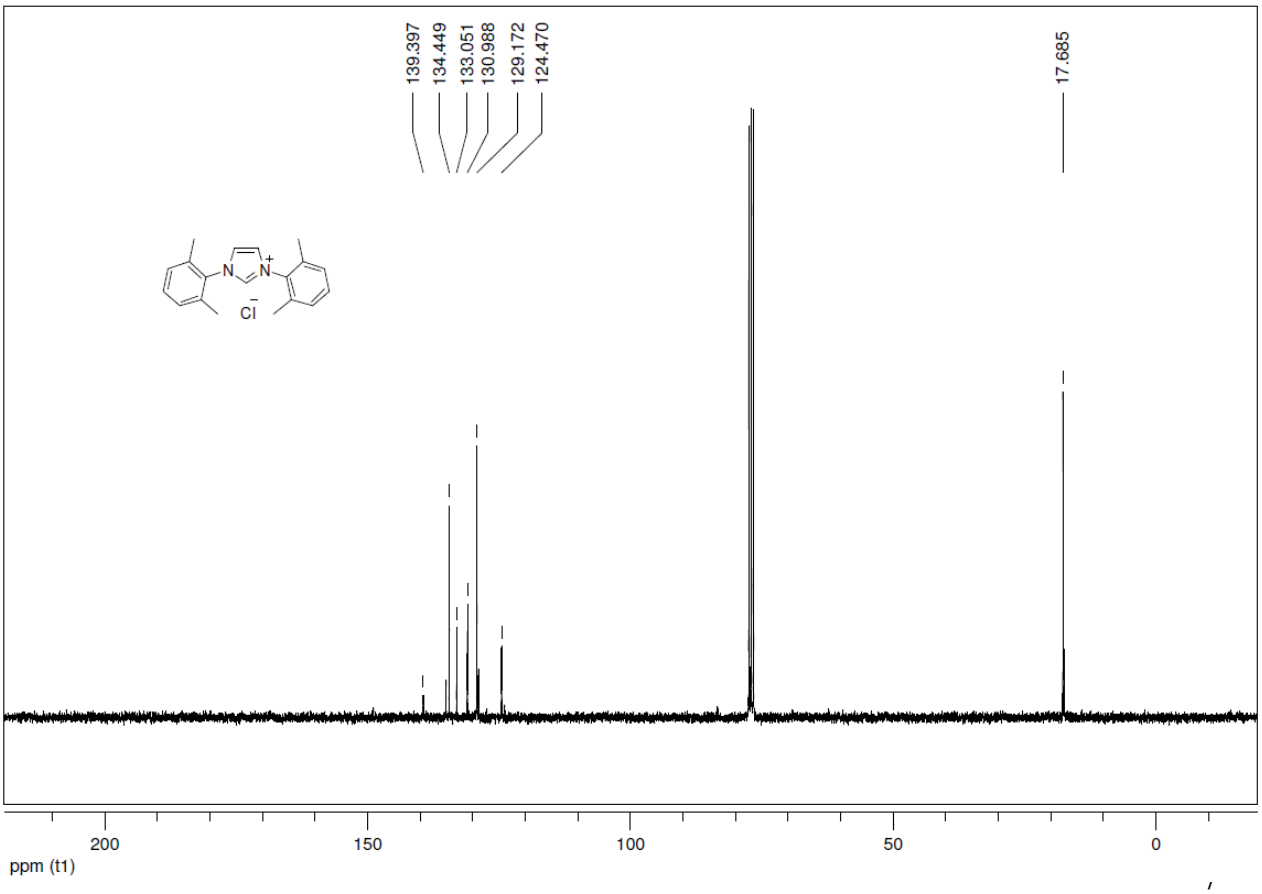

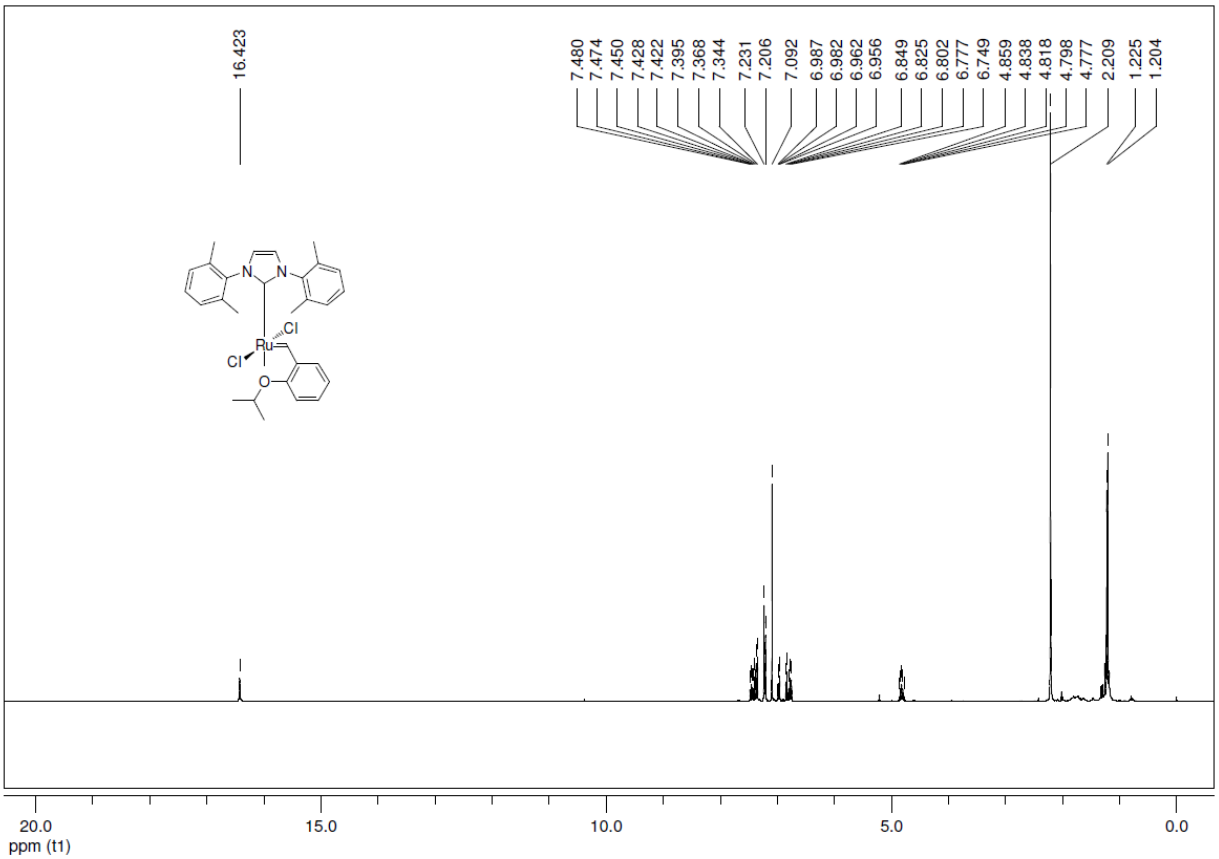
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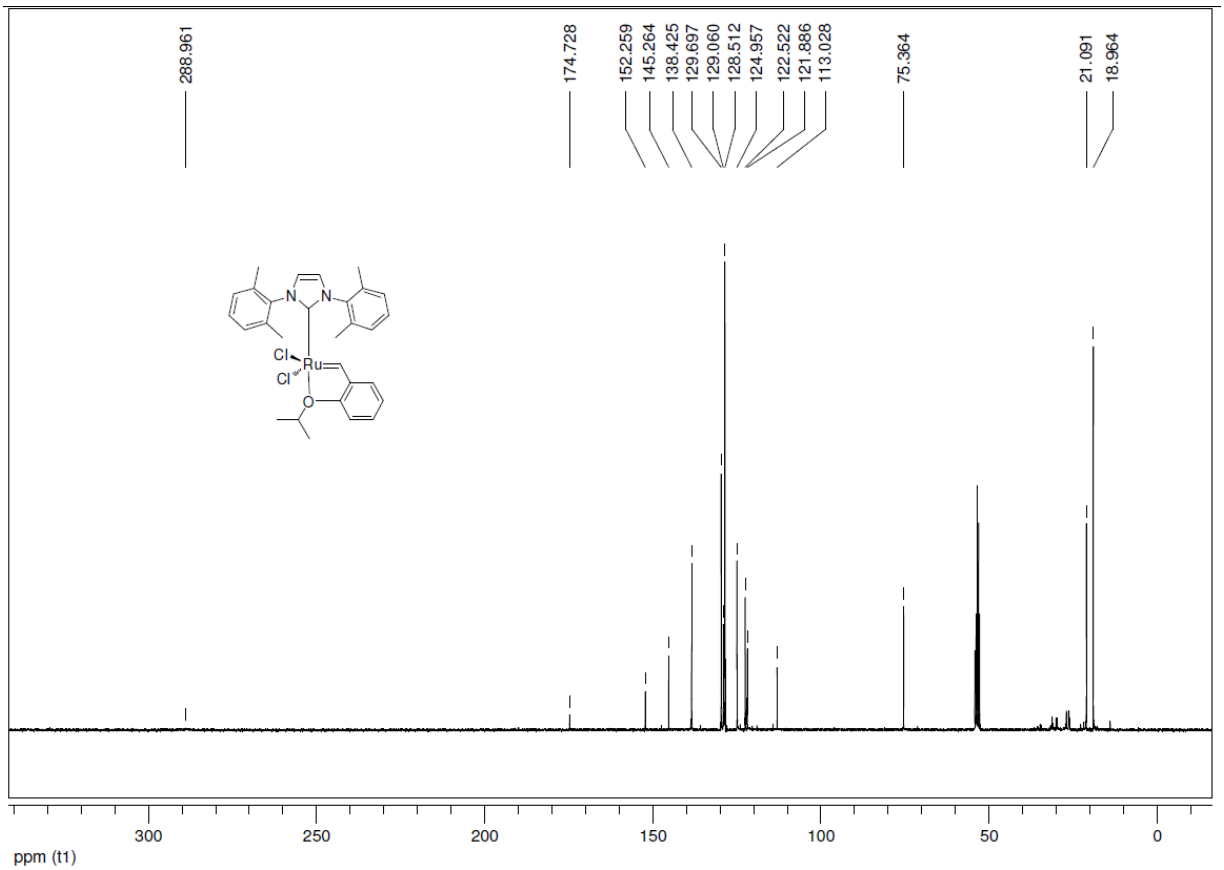
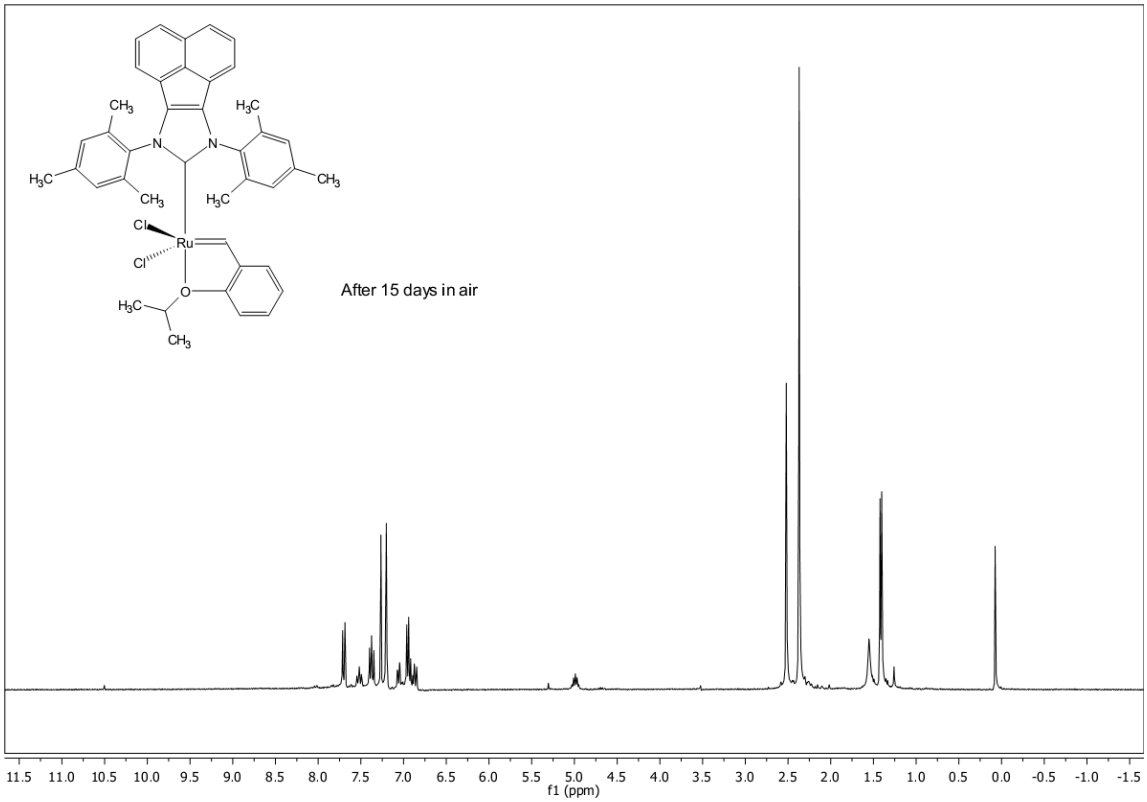
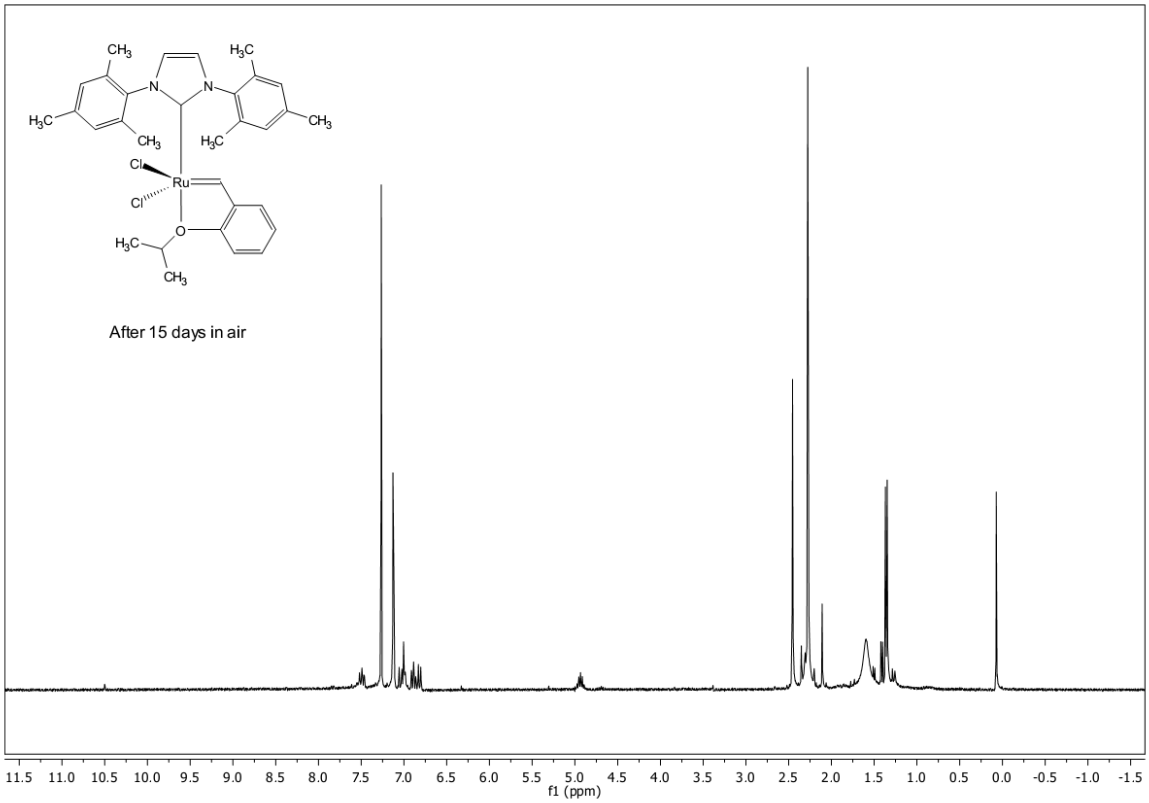
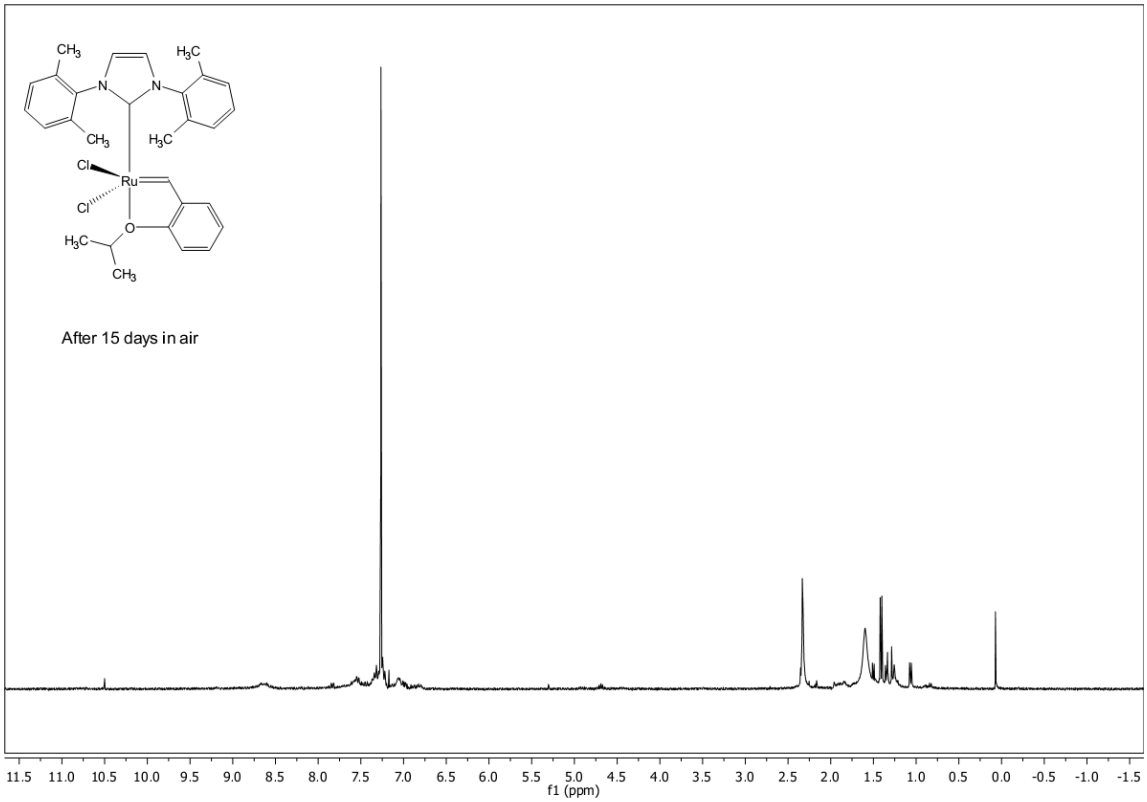
ppm (t1)


288.961
174.728
152.259
145.264
138.425
129.697
129.060
128.512
124.957
122.522
121.886
113.028
75.364
21.091
18.964
300
250
200
150
100
50
0
ppm (t1)

1H-NMRStability in air of the ruthenium complexes







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Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information Part 2- X Ray

Synthesis and characterization of new ruthenium *N*-heterocyclic carbene Hoveyda II-type complexes. Study of reactivity in ring closing metathesis reaction

Estíbaliz Merino,* Evelyne Poli, Urbano Díaz* and Daniel Brunel

Figure S1. ORTEP plot for 1,3-dimesityl-acenaphthylenyl-4,5-imidazolin-2-ylidene ruthenium isopropoxybenzylidene dichloride **3**

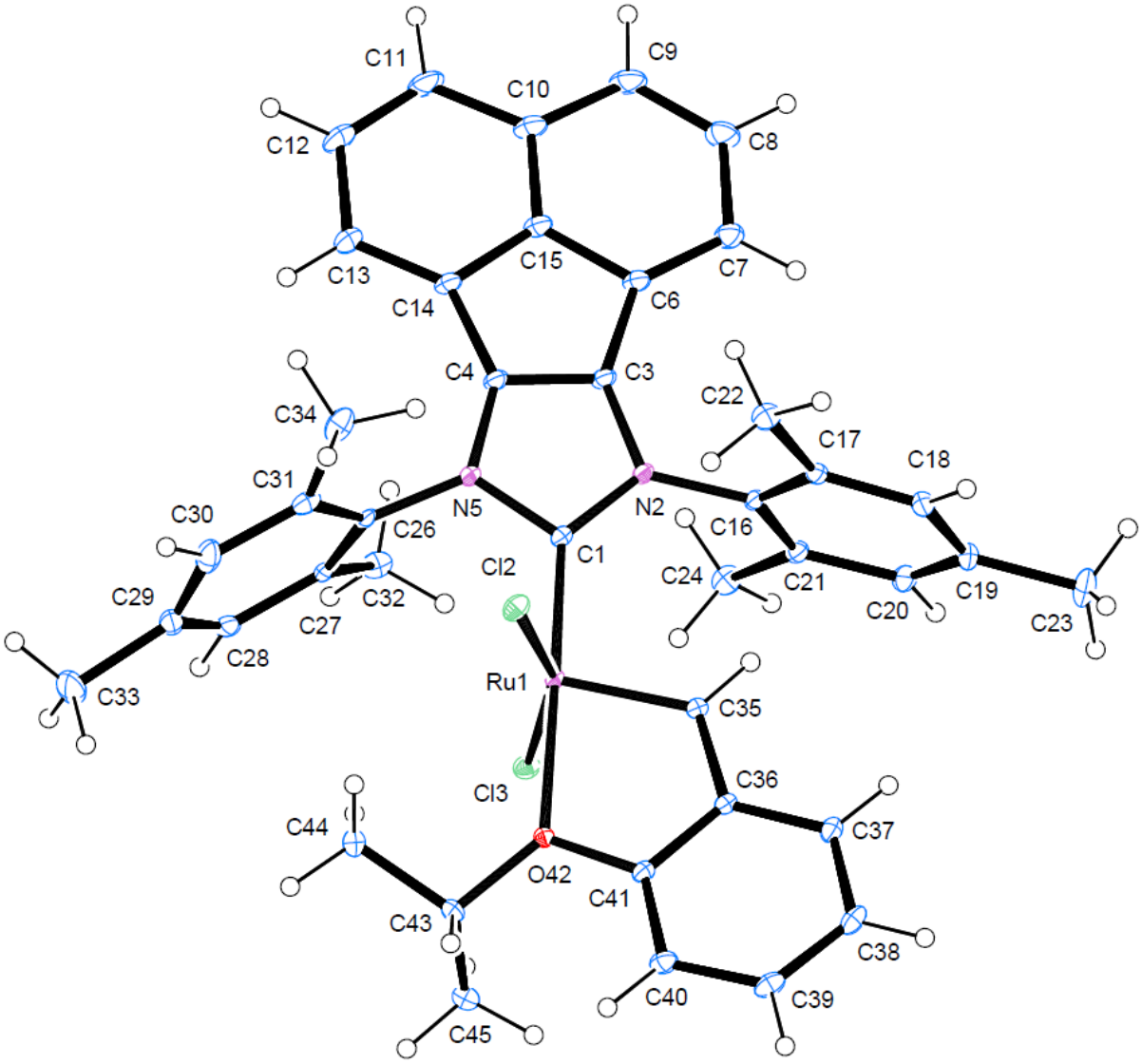

Table S1. Crystal data and structure refinement for **3**.

Identification code	cc01emm1n	
Empirical formula	$C_{41}H_{40}Cl_2N_2ORu$, 0.59(C_2H_5O), 0.41(CH_2Cl_2)	
Formula weight	801.10	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 20.7100(5) Å	α= 90°
	b = 10.3621(3) Å	β= 107.433(1)°
	c = 18.7711(4) Å	γ = 90°
Volume	3843.23(17) $Å^3$	
Z	4	
Density (calculated)	1.385 Mg/m^3	
Absorption coefficient	0.635 mm^{-1}	
F(000)	1654	
Crystal size	0.37 x 0.31 x 0.08 mm^3	
Theta range for data collection	2.06 to 30.51°	
Index ranges	-29<=h<=27, 0<=k<=14, 0<=l<=26	
Reflections collected	76624	
Independent reflections	11645 [R(int) = 0.0263]	
Completeness to theta = 30.51°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8959 and 0.7846	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11645 / 375 / 589	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0269, wR2 = 0.0622	
R indices (all data)	R1 = 0.0330, wR2 = 0.0650	
Largest diff. peak and hole	1.001 and -0.534 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	1566(1)	134(1)	2347(1)	11(1)
Cl(2)	1876(1)	-1517(1)	1668(1)	18(1)
Cl(3)	1306(1)	1154(1)	3345(1)	17(1)
C(1)	2462(1)	980(1)	2557(1)	13(1)
N(2)	2689(1)	2091(1)	2307(1)	13(1)
C(3)	3379(1)	2238(1)	2636(1)	15(1)
C(4)	3595(1)	1214(1)	3099(1)	15(1)
N(5)	3041(1)	445(1)	3051(1)	14(1)
C(6)	3936(1)	3129(1)	2682(1)	17(1)
C(7)	4034(1)	4288(2)	2378(1)	23(1)
C(8)	4697(1)	4835(2)	2606(1)	29(1)
C(9)	5236(1)	4237(2)	3105(1)	29(1)
C(10)	5148(1)	3034(2)	3431(1)	24(1)
C(11)	5646(1)	2297(2)	3965(1)	30(1)
C(12)	5479(1)	1163(2)	4238(1)	31(1)
C(13)	4806(1)	652(2)	4008(1)	24(1)
C(14)	4318(1)	1337(1)	3491(1)	18(1)
C(15)	4497(1)	2520(1)	3211(1)	18(1)
C(16)	2284(1)	2997(1)	1778(1)	13(1)
C(17)	2199(1)	2792(1)	1022(1)	15(1)
C(18)	1780(1)	3643(2)	514(1)	19(1)
C(19)	1473(1)	4683(2)	754(1)	22(1)
C(20)	1590(1)	4875(1)	1517(1)	21(1)
C(21)	1992(1)	4031(1)	2044(1)	16(1)
C(22)	2535(1)	1662(2)	772(1)	21(1)
C(23)	1028(1)	5605(2)	193(1)	36(1)
C(24)	2092(1)	4201(2)	2866(1)	22(1)
C(26)	3010(9)	-577(8)	3541(6)	14(1)
C(27)	2899(6)	-252(7)	4224(4)	15(1)
C(28)	2784(4)	-1265(7)	4660(4)	23(1)
C(29)	2823(3)	-2541(7)	4465(4)	26(1)
C(30)	3032(5)	-2817(7)	3847(5)	28(1)

C(31)	3133(6)	-1847(8)	3373(5)	21(1)
C(32)	2946(6)	1117(7)	4486(5)	21(1)
C(33)	2648(3)	-3627(8)	4915(4)	44(2)
C(34)	3414(7)	-2176(12)	2740(6)	27(1)
C(76)	3053(14)	-740(14)	3504(10)	18(2)
C(77)	2914(10)	-563(14)	4182(8)	26(2)
C(78)	2847(7)	-1672(17)	4573(7)	35(2)
C(79)	2925(9)	-2870(14)	4316(7)	42(3)
C(80)	3117(10)	-2987(12)	3678(9)	38(3)
C(81)	3195(9)	-1928(9)	3248(8)	19(2)
C(82)	2906(9)	761(16)	4497(9)	31(2)
C(83)	2834(12)	-4063(17)	4746(8)	84(6)
C(84)	3446(11)	-2072(19)	2584(10)	31(2)
C(35)	1054(1)	1113(1)	1569(1)	14(1)
C(36)	365(1)	710(1)	1199(1)	13(1)
C(37)	-56(1)	1328(1)	563(1)	16(1)
C(38)	-701(1)	863(2)	217(1)	20(1)
C(39)	-929(1)	-224(2)	504(1)	21(1)
C(40)	-530(1)	-857(1)	1139(1)	18(1)
C(41)	115(1)	-374(1)	1480(1)	14(1)
O(42)	576(1)	-893(1)	2101(1)	15(1)
C(43)	343(1)	-1832(1)	2560(1)	18(1)
C(44)	980(1)	-2414(2)	3085(1)	22(1)
C(45)	-100(1)	-1150(2)	2956(1)	23(1)
C(50)	4767(5)	1601(9)	434(6)	50(2)
Cl(51)	4491(1)	2572(1)	1071(1)	41(1)
Cl(52)	4059(1)	813(2)	-197(1)	58(1)
O(60)	5000	0	0	79(1)
C(61)	5240(5)	1082(11)	491(5)	76(2)
C(62)	4885(9)	1965(17)	612(13)	98(5)
C(63)	5432(5)	-962(11)	-118(7)	73(2)
C(64)	5387(9)	-1870(20)	-583(13)	83(4)

Table S3. Bond lengths [Å] for **3**.

Atom-atom	Distance
Ru(1)-C(35)	1.8341(13)
Ru(1)-C(1)	1.9820(13)
Ru(1)-O(42)	2.2333(9)
Ru(1)-Cl(2)	2.3346(3)
Ru(1)-Cl(3)	2.3504(3)
C(1)-N(2)	1.3778(17)
C(1)-N(5)	1.3923(16)
N(2)-C(3)	1.3832(16)
N(2)-C(16)	1.4397(16)
C(3)-C(4)	1.3595(19)
C(3)-C(6)	1.4601(19)
C(4)-N(5)	1.3780(17)
C(4)-C(14)	1.4621(18)
N(5)-C(26)	1.417(10)
N(5)-C(76)	1.490(14)
C(6)-C(7)	1.370(2)
C(6)-C(15)	1.429(2)
C(7)-C(8)	1.428(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.371(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.424(2)
C(9)-H(9)	0.9500
C(10)-C(15)	1.3930(19)
C(10)-C(11)	1.426(2)
C(11)-C(12)	1.368(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.431(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.371(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.426(2)
C(16)-C(17)	1.3935(19)
C(16)-C(21)	1.3944(19)
C(17)-C(18)	1.3948(19)
C(17)-C(22)	1.507(2)

C(18)-C(19)	1.393(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.393(2)
C(19)-C(23)	1.512(2)
C(20)-C(21)	1.395(2)
C(20)-H(20)	0.9500
C(21)-C(24)	1.504(2)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(26)-C(31)	1.395(7)
C(26)-C(27)	1.409(7)
C(27)-C(28)	1.396(6)
C(27)-C(32)	1.495(6)
C(28)-C(29)	1.382(6)
C(28)-H(28)	0.9500
C(29)-C(30)	1.384(6)
C(29)-C(33)	1.515(6)
C(30)-C(31)	1.399(7)
C(30)-H(30)	0.9500
C(31)-C(34)	1.509(7)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(76)-C(81)	1.384(10)
C(76)-C(77)	1.397(11)
C(77)-C(78)	1.394(10)

C(77)-C(82)	1.496(10)
C(78)-C(79)	1.359(10)
C(78)-H(78)	0.9500
C(79)-C(80)	1.374(10)
C(79)-C(83)	1.519(9)
C(80)-C(81)	1.400(10)
C(80)-H(80)	0.9500
C(81)-C(84)	1.496(10)
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(83)-H(83A)	0.9800
C(83)-H(83B)	0.9800
C(83)-H(83C)	0.9800
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(35)-C(36)	1.4480(18)
C(35)-H(35)	0.9500
C(36)-C(41)	1.4033(19)
C(36)-C(37)	1.4051(18)
C(37)-C(38)	1.385(2)
C(37)-H(37)	0.9500
C(38)-C(39)	1.390(2)
C(38)-H(38)	0.9500
C(39)-C(40)	1.394(2)
C(39)-H(39)	0.9500
C(40)-C(41)	1.3889(18)
C(40)-H(40)	0.9500
C(41)-O(42)	1.3758(16)
O(42)-C(43)	1.4728(16)
C(43)-C(44)	1.516(2)
C(43)-C(45)	1.518(2)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800

C(45)-H(45C)	0.9800
C(50)-Cl(51)	1.782(7)
C(50)-Cl(52)	1.784(9)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
O(60)-C(63)	1.401(12)
O(60)-C(61)	1.441(11)
C(61)-C(62)	1.237(15)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-C(64)	1.265(15)
C(63)-H(63A)	0.9900
C(63)-H(63B)	0.9900
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800

Table S4. Angles [°] for **3**.

Atom-atom-atom	Angle
C(35)-Ru(1)-C(1)	101.38(6)
C(35)-Ru(1)-O(42)	79.72(5)
C(1)-Ru(1)-O(42)	177.71(5)
C(35)-Ru(1)-Cl(2)	99.09(4)
C(1)-Ru(1)-Cl(2)	92.22(4)
O(42)-Ru(1)-Cl(2)	85.61(3)
C(35)-Ru(1)-Cl(3)	99.79(4)
C(1)-Ru(1)-Cl(3)	93.87(4)
O(42)-Ru(1)-Cl(3)	87.91(3)
Cl(2)-Ru(1)-Cl(3)	158.585(13)
N(2)-C(1)-N(5)	104.19(11)
N(2)-C(1)-Ru(1)	134.20(9)
N(5)-C(1)-Ru(1)	121.60(10)
C(1)-N(2)-C(3)	110.64(11)
C(1)-N(2)-C(16)	126.26(11)
C(3)-N(2)-C(16)	123.10(11)
C(4)-C(3)-N(2)	107.33(12)
C(4)-C(3)-C(6)	110.62(12)
N(2)-C(3)-C(6)	141.97(13)
C(3)-C(4)-N(5)	107.49(11)
C(3)-C(4)-C(14)	110.24(12)
N(5)-C(4)-C(14)	142.20(13)
C(4)-N(5)-C(1)	110.34(11)
C(4)-N(5)-C(26)	126.1(7)
C(1)-N(5)-C(26)	122.2(7)
C(4)-N(5)-C(76)	124.6(11)
C(1)-N(5)-C(76)	124.9(11)
C(26)-N(5)-C(76)	7.9(9)
C(7)-C(6)-C(15)	119.00(13)
C(7)-C(6)-C(3)	137.99(14)
C(15)-C(6)-C(3)	103.00(12)
C(6)-C(7)-C(8)	118.24(15)
C(6)-C(7)-H(7)	120.9
C(8)-C(7)-H(7)	120.9
C(9)-C(8)-C(7)	122.51(15)
C(9)-C(8)-H(8)	118.7

C(7)-C(8)-H(8)	118.7
C(8)-C(9)-C(10)	120.47(14)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(15)-C(10)-C(9)	116.35(14)
C(15)-C(10)-C(11)	115.92(15)
C(9)-C(10)-C(11)	127.73(14)
C(12)-C(11)-C(10)	120.75(14)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	122.62(15)
C(11)-C(12)-H(12)	118.7
C(13)-C(12)-H(12)	118.7
C(14)-C(13)-C(12)	117.79(15)
C(14)-C(13)-H(13)	121.1
C(12)-C(13)-H(13)	121.1
C(13)-C(14)-C(15)	119.27(13)
C(13)-C(14)-C(4)	137.53(14)
C(15)-C(14)-C(4)	103.20(12)
C(10)-C(15)-C(14)	123.65(14)
C(10)-C(15)-C(6)	123.42(14)
C(14)-C(15)-C(6)	112.93(12)
C(17)-C(16)-C(21)	123.10(12)
C(17)-C(16)-N(2)	118.20(12)
C(21)-C(16)-N(2)	118.70(12)
C(16)-C(17)-C(18)	117.56(13)
C(16)-C(17)-C(22)	120.43(12)
C(18)-C(17)-C(22)	121.99(13)
C(19)-C(18)-C(17)	121.29(14)
C(19)-C(18)-H(18)	119.4
C(17)-C(18)-H(18)	119.4
C(20)-C(19)-C(18)	119.13(13)
C(20)-C(19)-C(23)	120.52(15)
C(18)-C(19)-C(23)	120.34(15)
C(19)-C(20)-C(21)	121.57(14)
C(19)-C(20)-H(20)	119.2
C(21)-C(20)-H(20)	119.2
C(16)-C(21)-C(20)	117.29(13)
C(16)-C(21)-C(24)	121.10(12)

C(20)-C(21)-C(24)	121.59(13)
C(17)-C(22)-H(22A)	109.5
C(17)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(17)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(19)-C(23)-H(23A)	109.5
C(19)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(19)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(31)-C(26)-C(27)	121.5(7)
C(31)-C(26)-N(5)	120.7(6)
C(27)-C(26)-N(5)	117.6(6)
C(28)-C(27)-C(26)	117.2(6)
C(28)-C(27)-C(32)	121.7(5)
C(26)-C(27)-C(32)	121.0(6)
C(29)-C(28)-C(27)	122.0(5)
C(29)-C(28)-H(28)	119.0
C(27)-C(28)-H(28)	119.0
C(28)-C(29)-C(30)	118.6(5)
C(28)-C(29)-C(33)	121.3(5)
C(30)-C(29)-C(33)	120.1(5)
C(29)-C(30)-C(31)	121.9(5)
C(29)-C(30)-H(30)	119.0
C(31)-C(30)-H(30)	119.0
C(26)-C(31)-C(30)	117.5(6)
C(26)-C(31)-C(34)	122.1(7)
C(30)-C(31)-C(34)	120.3(7)
C(81)-C(76)-C(77)	123.7(10)
C(81)-C(76)-N(5)	120.3(9)

C(77)-C(76)-N(5)	116.0(9)
C(78)-C(77)-C(76)	116.9(9)
C(78)-C(77)-C(82)	122.2(10)
C(76)-C(77)-C(82)	120.7(10)
C(79)-C(78)-C(77)	121.6(8)
C(79)-C(78)-H(78)	119.2
C(77)-C(78)-H(78)	119.2
C(78)-C(79)-C(80)	119.1(8)
C(78)-C(79)-C(83)	120.4(9)
C(80)-C(79)-C(83)	120.4(9)
C(79)-C(80)-C(81)	123.1(9)
C(79)-C(80)-H(80)	118.5
C(81)-C(80)-H(80)	118.5
C(76)-C(81)-C(80)	115.1(9)
C(76)-C(81)-C(84)	122.8(10)
C(80)-C(81)-C(84)	122.1(9)
C(77)-C(82)-H(82A)	109.5
C(77)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5
C(77)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(79)-C(83)-H(83A)	109.5
C(79)-C(83)-H(83B)	109.5
H(83A)-C(83)-H(83B)	109.5
C(79)-C(83)-H(83C)	109.5
H(83A)-C(83)-H(83C)	109.5
H(83B)-C(83)-H(83C)	109.5
C(81)-C(84)-H(84A)	109.5
C(81)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(81)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(36)-C(35)-Ru(1)	118.33(10)
C(36)-C(35)-H(35)	120.8
Ru(1)-C(35)-H(35)	120.8
C(41)-C(36)-C(37)	118.63(12)
C(41)-C(36)-C(35)	118.17(12)

C(37)-C(36)-C(35)	123.17(13)
C(38)-C(37)-C(36)	120.34(13)
C(38)-C(37)-H(37)	119.8
C(36)-C(37)-H(37)	119.8
C(37)-C(38)-C(39)	119.46(13)
C(37)-C(38)-H(38)	120.3
C(39)-C(38)-H(38)	120.3
C(38)-C(39)-C(40)	121.95(13)
C(38)-C(39)-H(39)	119.0
C(40)-C(39)-H(39)	119.0
C(41)-C(40)-C(39)	117.77(14)
C(41)-C(40)-H(40)	121.1
C(39)-C(40)-H(40)	121.1
O(42)-C(41)-C(40)	125.16(13)
O(42)-C(41)-C(36)	113.00(11)
C(40)-C(41)-C(36)	121.82(13)
C(41)-O(42)-C(43)	119.28(10)
C(41)-O(42)-Ru(1)	110.50(8)
C(43)-O(42)-Ru(1)	129.37(8)
O(42)-C(43)-C(44)	105.70(11)
O(42)-C(43)-C(45)	109.33(11)
C(44)-C(43)-C(45)	113.72(13)
O(42)-C(43)-H(43)	109.3
C(44)-C(43)-H(43)	109.3
C(45)-C(43)-H(43)	109.3
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
Cl(51)-C(50)-Cl(52)	109.8(4)
Cl(51)-C(50)-H(50A)	109.7

Cl(52)-C(50)-H(50A)	109.7
Cl(51)-C(50)-H(50B)	109.7
Cl(52)-C(50)-H(50B)	109.7
H(50A)-C(50)-H(50B)	108.2
C(63)-O(60)-C(61)	122.7(6)
C(62)-C(61)-O(60)	125.7(12)
C(62)-C(61)-H(61A)	105.9
O(60)-C(61)-H(61A)	105.9
C(62)-C(61)-H(61B)	105.9
O(60)-C(61)-H(61B)	105.9
H(61A)-C(61)-H(61B)	106.2
C(61)-C(62)-H(62A)	109.5
C(61)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(61)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(64)-C(63)-O(60)	135.9(12)
C(64)-C(63)-H(63A)	103.2
O(60)-C(63)-H(63A)	103.2
C(64)-C(63)-H(63B)	103.2
O(60)-C(63)-H(63B)	103.2
H(63A)-C(63)-H(63B)	105.2
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5

Table S5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	9(1)	12(1)	12(1)	1(1)	2(1)	1(1)
Cl(2)	17(1)	18(1)	19(1)	-3(1)	3(1)	3(1)
Cl(3)	15(1)	20(1)	16(1)	-2(1)	5(1)	1(1)
C(1)	11(1)	14(1)	13(1)	0(1)	3(1)	2(1)
N(2)	10(1)	13(1)	16(1)	1(1)	2(1)	1(1)
C(3)	10(1)	15(1)	20(1)	0(1)	3(1)	0(1)
C(4)	10(1)	16(1)	19(1)	0(1)	3(1)	0(1)
N(5)	10(1)	15(1)	16(1)	2(1)	2(1)	1(1)
C(6)	12(1)	16(1)	23(1)	-2(1)	5(1)	-1(1)
C(7)	17(1)	18(1)	32(1)	0(1)	6(1)	-1(1)
C(8)	22(1)	20(1)	45(1)	0(1)	12(1)	-7(1)
C(9)	16(1)	27(1)	43(1)	-4(1)	8(1)	-7(1)
C(10)	13(1)	26(1)	32(1)	-4(1)	5(1)	-3(1)
C(11)	11(1)	37(1)	37(1)	-2(1)	-1(1)	-3(1)
C(12)	12(1)	40(1)	34(1)	5(1)	-4(1)	2(1)
C(13)	14(1)	29(1)	26(1)	4(1)	1(1)	1(1)
C(14)	10(1)	21(1)	21(1)	-1(1)	3(1)	0(1)
C(15)	12(1)	19(1)	23(1)	-2(1)	4(1)	-1(1)
C(16)	10(1)	12(1)	17(1)	2(1)	2(1)	0(1)
C(17)	13(1)	14(1)	19(1)	1(1)	5(1)	-2(1)
C(18)	18(1)	22(1)	18(1)	5(1)	4(1)	-1(1)
C(19)	19(1)	19(1)	26(1)	10(1)	5(1)	3(1)
C(20)	19(1)	14(1)	29(1)	4(1)	8(1)	4(1)
C(21)	13(1)	13(1)	21(1)	0(1)	5(1)	-1(1)
C(22)	21(1)	21(1)	20(1)	-3(1)	7(1)	1(1)
C(23)	35(1)	34(1)	36(1)	18(1)	6(1)	14(1)
C(24)	22(1)	19(1)	23(1)	-4(1)	6(1)	2(1)
C(26)	7(3)	12(2)	21(2)	3(2)	-1(2)	1(2)
C(27)	8(1)	23(2)	14(2)	7(2)	1(1)	2(2)
C(28)	11(1)	37(3)	21(2)	9(2)	2(1)	0(2)
C(29)	13(2)	31(3)	29(3)	14(2)	-2(1)	-6(2)
C(30)	23(2)	19(2)	33(4)	7(2)	-4(2)	-4(2)
C(31)	12(2)	26(2)	22(2)	-1(2)	1(2)	1(1)
C(32)	18(2)	26(2)	19(2)	-6(2)	4(1)	0(2)

C(33)	26(2)	48(3)	49(3)	26(2)	-2(2)	-16(2)
C(34)	26(2)	23(2)	29(3)	-1(2)	2(2)	9(2)
C(76)	9(3)	23(5)	21(4)	15(3)	4(3)	3(4)
C(77)	11(3)	30(5)	33(4)	3(3)	-1(2)	0(4)
C(78)	21(4)	58(6)	21(3)	21(4)	-3(2)	-13(5)
C(79)	44(6)	36(5)	29(5)	17(4)	-14(3)	-25(4)
C(80)	42(7)	22(4)	31(5)	10(3)	-18(3)	-13(3)
C(81)	16(4)	5(3)	29(5)	9(2)	-4(3)	-2(2)
C(82)	18(3)	50(6)	22(3)	4(5)	1(2)	5(5)
C(83)	116(11)	65(7)	44(5)	34(5)	-18(6)	-61(7)
C(84)	26(3)	21(4)	42(7)	-6(4)	4(4)	9(3)
C(35)	11(1)	14(1)	15(1)	1(1)	4(1)	1(1)
C(36)	11(1)	14(1)	13(1)	-1(1)	3(1)	2(1)
C(37)	16(1)	17(1)	14(1)	1(1)	4(1)	4(1)
C(38)	17(1)	23(1)	15(1)	-3(1)	-1(1)	6(1)
C(39)	13(1)	25(1)	21(1)	-6(1)	0(1)	0(1)
C(40)	13(1)	19(1)	21(1)	-2(1)	3(1)	-2(1)
C(41)	11(1)	16(1)	14(1)	0(1)	2(1)	1(1)
O(42)	10(1)	17(1)	16(1)	5(1)	1(1)	-2(1)
C(43)	16(1)	16(1)	22(1)	5(1)	6(1)	-3(1)
C(44)	20(1)	21(1)	25(1)	9(1)	7(1)	3(1)
C(45)	19(1)	28(1)	25(1)	7(1)	10(1)	0(1)
C(50)	65(5)	37(4)	69(5)	-11(3)	52(4)	-21(3)
Cl(51)	43(1)	29(1)	46(1)	-6(1)	7(1)	4(1)
Cl(52)	63(1)	59(1)	53(1)	-20(1)	19(1)	-7(1)
O(60)	75(3)	77(3)	77(3)	40(2)	11(2)	-6(2)
C(61)	57(4)	107(5)	52(4)	30(3)	-3(3)	2(3)
C(62)	94(11)	59(6)	116(9)	43(5)	-7(9)	11(7)
C(63)	53(4)	82(4)	79(5)	37(3)	13(4)	-18(3)
C(64)	66(8)	89(8)	86(9)	32(5)	10(8)	-6(6)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(7)	3671	4715	2025	27
H(8)	4768	5645	2405	34
H(9)	5670	4628	3235	35
H(11)	6100	2598	4134	36
H(12)	5822	695	4593	37
H(13)	4701	-136	4208	29
H(18)	1702	3510	-6	23
H(20)	1392	5599	1682	25
H(22A)	3025	1707	1010	31
H(22B)	2438	1688	228	31
H(22C)	2360	856	916	31
H(23A)	697	5998	406	54
H(23B)	790	5132	-262	54
H(23C)	1309	6281	72	54
H(24A)	1926	5054	2955	32
H(24B)	2574	4128	3140	32
H(24C)	1839	3532	3038	32
H(28)	2675	-1071	5105	28
H(30)	3109	-3690	3741	33
H(32A)	2929	1143	5002	32
H(32B)	2566	1612	4166	32
H(32C)	3373	1494	4463	32
H(33A)	2598	-3281	5381	66
H(33B)	3011	-4272	5029	66
H(33C)	2223	-4031	4625	66
H(34A)	3350	-1442	2397	41
H(34B)	3177	-2931	2471	41
H(34C)	3898	-2369	2942	41
H(78)	2743	-1589	5031	42
H(80)	3199	-3827	3521	46
H(82A)	3346	1174	4568	46
H(82B)	2814	699	4978	46
H(82C)	2551	1276	4151	46

H(83A)	2795	-3805	5234	126
H(83B)	3225	-4633	4817	126
H(83C)	2422	-4519	4464	126
H(84A)	3186	-1504	2183	47
H(84B)	3389	-2970	2411	47
H(84C)	3926	-1838	2721	47
H(35)	1235	1865	1412	16
H(37)	102	2070	368	19
H(38)	-986	1284	-213	23
H(39)	-1369	-545	260	25
H(40)	-693	-1594	1332	22
H(43)	74	-2524	2231	21
H(44A)	1261	-2768	2795	33
H(44B)	857	-3106	3377	33
H(44C)	1234	-1746	3424	33
H(45A)	167	-491	3292	35
H(45B)	-270	-1779	3246	35
H(45C)	-482	-739	2587	35
H(50A)	5096	950	714	60
H(50B)	4996	2150	151	60
H(61A)	5478	708	985	91
H(61B)	5591	1504	312	91
H(62A)	4451	1982	216	147
H(62B)	5118	2791	622	147
H(62C)	4804	1822	1094	147
H(63A)	5831	-469	-153	87
H(63B)	5584	-1409	370	87
H(64A)	5530	-2679	-314	124
H(64B)	5678	-1678	-896	124
H(64C)	4916	-1946	-898	124

Table S7. Torsion angles [°] for **3**.

C(35)-Ru(1)-C(1)-N(2)	8.25(14)
O(42)-Ru(1)-C(1)-N(2)	126.8(11)
Cl(2)-Ru(1)-C(1)-N(2)	107.99(13)
Cl(3)-Ru(1)-C(1)-N(2)	-92.56(13)
C(35)-Ru(1)-C(1)-N(5)	-171.20(11)
O(42)-Ru(1)-C(1)-N(5)	-52.7(12)
Cl(2)-Ru(1)-C(1)-N(5)	-71.46(10)
Cl(3)-Ru(1)-C(1)-N(5)	88.00(10)
N(5)-C(1)-N(2)-C(3)	-0.33(15)
Ru(1)-C(1)-N(2)-C(3)	-179.85(11)
N(5)-C(1)-N(2)-C(16)	179.68(12)
Ru(1)-C(1)-N(2)-C(16)	0.2(2)
C(1)-N(2)-C(3)-C(4)	0.19(16)
C(16)-N(2)-C(3)-C(4)	-179.82(12)
C(1)-N(2)-C(3)-C(6)	-176.04(18)
C(16)-N(2)-C(3)-C(6)	3.9(3)
N(2)-C(3)-C(4)-N(5)	0.04(16)
C(6)-C(3)-C(4)-N(5)	177.56(12)
N(2)-C(3)-C(4)-C(14)	-177.61(12)
C(6)-C(3)-C(4)-C(14)	-0.09(17)
C(3)-C(4)-N(5)-C(1)	-0.25(16)
C(14)-C(4)-N(5)-C(1)	176.14(18)
C(3)-C(4)-N(5)-C(26)	-166.8(4)
C(14)-C(4)-N(5)-C(26)	9.5(5)
C(3)-C(4)-N(5)-C(76)	-176.3(7)
C(14)-C(4)-N(5)-C(76)	0.1(7)
N(2)-C(1)-N(5)-C(4)	0.36(15)
Ru(1)-C(1)-N(5)-C(4)	179.95(10)
N(2)-C(1)-N(5)-C(26)	167.6(4)
Ru(1)-C(1)-N(5)-C(26)	-12.8(4)
N(2)-C(1)-N(5)-C(76)	176.4(7)
Ru(1)-C(1)-N(5)-C(76)	-4.0(7)
C(4)-C(3)-C(6)-C(7)	-178.67(18)
N(2)-C(3)-C(6)-C(7)	-2.5(3)
C(4)-C(3)-C(6)-C(15)	0.30(16)
N(2)-C(3)-C(6)-C(15)	176.46(18)
C(15)-C(6)-C(7)-C(8)	0.0(2)

C(3)-C(6)-C(7)-C(8)	178.90(17)
C(6)-C(7)-C(8)-C(9)	1.0(3)
C(7)-C(8)-C(9)-C(10)	-1.2(3)
C(8)-C(9)-C(10)-C(15)	0.3(3)
C(8)-C(9)-C(10)-C(11)	-178.78(18)
C(15)-C(10)-C(11)-C(12)	-0.4(3)
C(9)-C(10)-C(11)-C(12)	178.71(18)
C(10)-C(11)-C(12)-C(13)	0.1(3)
C(11)-C(12)-C(13)-C(14)	0.4(3)
C(12)-C(13)-C(14)-C(15)	-0.5(2)
C(12)-C(13)-C(14)-C(4)	179.60(17)
C(3)-C(4)-C(14)-C(13)	179.71(18)
N(5)-C(4)-C(14)-C(13)	3.4(4)
C(3)-C(4)-C(14)-C(15)	-0.16(16)
N(5)-C(4)-C(14)-C(15)	-176.50(19)
C(9)-C(10)-C(15)-C(14)	-178.95(15)
C(11)-C(10)-C(15)-C(14)	0.2(2)
C(9)-C(10)-C(15)-C(6)	0.8(2)
C(11)-C(10)-C(15)-C(6)	179.97(15)
C(13)-C(14)-C(15)-C(10)	0.2(2)
C(4)-C(14)-C(15)-C(10)	-179.87(15)
C(13)-C(14)-C(15)-C(6)	-179.53(14)
C(4)-C(14)-C(15)-C(6)	0.37(17)
C(7)-C(6)-C(15)-C(10)	-1.0(2)
C(3)-C(6)-C(15)-C(10)	179.82(14)
C(7)-C(6)-C(15)-C(14)	178.80(14)
C(3)-C(6)-C(15)-C(14)	-0.42(17)
C(1)-N(2)-C(16)-C(17)	-89.04(16)
C(3)-N(2)-C(16)-C(17)	90.98(16)
C(1)-N(2)-C(16)-C(21)	90.54(16)
C(3)-N(2)-C(16)-C(21)	-89.45(16)
C(21)-C(16)-C(17)-C(18)	-2.5(2)
N(2)-C(16)-C(17)-C(18)	177.06(12)
C(21)-C(16)-C(17)-C(22)	179.37(13)
N(2)-C(16)-C(17)-C(22)	-1.07(19)
C(16)-C(17)-C(18)-C(19)	1.9(2)
C(22)-C(17)-C(18)-C(19)	179.99(14)
C(17)-C(18)-C(19)-C(20)	0.2(2)
C(17)-C(18)-C(19)-C(23)	179.10(15)

C(18)-C(19)-C(20)-C(21)	-1.8(2)
C(23)-C(19)-C(20)-C(21)	179.27(15)
C(17)-C(16)-C(21)-C(20)	1.0(2)
N(2)-C(16)-C(21)-C(20)	-178.60(12)
C(17)-C(16)-C(21)-C(24)	179.18(13)
N(2)-C(16)-C(21)-C(24)	-0.37(19)
C(19)-C(20)-C(21)-C(16)	1.3(2)
C(19)-C(20)-C(21)-C(24)	-176.97(14)
C(4)-N(5)-C(26)-C(31)	-94.4(14)
C(1)-N(5)-C(26)-C(31)	100.4(14)
C(76)-N(5)-C(26)-C(31)	-12(12)
C(4)-N(5)-C(26)-C(27)	81.1(14)
C(1)-N(5)-C(26)-C(27)	-84.0(13)
C(76)-N(5)-C(26)-C(27)	163(14)
C(31)-C(26)-C(27)-C(28)	-12(2)
N(5)-C(26)-C(27)-C(28)	172.1(10)
C(31)-C(26)-C(27)-C(32)	164.0(13)
N(5)-C(26)-C(27)-C(32)	-11.5(19)
C(26)-C(27)-C(28)-C(29)	4.6(15)
C(32)-C(27)-C(28)-C(29)	-171.8(8)
C(27)-C(28)-C(29)-C(30)	4.8(12)
C(27)-C(28)-C(29)-C(33)	-175.6(8)
C(28)-C(29)-C(30)-C(31)	-7.0(14)
C(33)-C(29)-C(30)-C(31)	173.5(9)
C(27)-C(26)-C(31)-C(30)	10(2)
N(5)-C(26)-C(31)-C(30)	-174.2(12)
C(27)-C(26)-C(31)-C(34)	-165.1(13)
N(5)-C(26)-C(31)-C(34)	10(2)
C(29)-C(30)-C(31)-C(26)	-0.5(18)
C(29)-C(30)-C(31)-C(34)	175.1(10)
C(4)-N(5)-C(76)-C(81)	-89(2)
C(1)-N(5)-C(76)-C(81)	95(2)
C(26)-N(5)-C(76)-C(81)	167(15)
C(4)-N(5)-C(76)-C(77)	91(2)
C(1)-N(5)-C(76)-C(77)	-85(2)
C(26)-N(5)-C(76)-C(77)	-13(11)
C(81)-C(76)-C(77)-C(78)	-7(4)
N(5)-C(76)-C(77)-C(78)	172.9(17)
C(81)-C(76)-C(77)-C(82)	167(2)

N(5)-C(76)-C(77)-C(82)	-13(3)
C(76)-C(77)-C(78)-C(79)	1(3)
C(82)-C(77)-C(78)-C(79)	-173.1(14)
C(77)-C(78)-C(79)-C(80)	4(2)
C(77)-C(78)-C(79)-C(83)	-178.7(14)
C(78)-C(79)-C(80)-C(81)	-4(2)
C(83)-C(79)-C(80)-C(81)	178.6(14)
C(77)-C(76)-C(81)-C(80)	7(3)
N(5)-C(76)-C(81)-C(80)	-173.0(18)
C(77)-C(76)-C(81)-C(84)	-170(2)
N(5)-C(76)-C(81)-C(84)	10(3)
C(79)-C(80)-C(81)-C(76)	-1(3)
C(79)-C(80)-C(81)-C(84)	176.1(17)
C(1)-Ru(1)-C(35)-C(36)	173.82(10)
O(42)-Ru(1)-C(35)-C(36)	-4.14(10)
Cl(2)-Ru(1)-C(35)-C(36)	79.67(10)
Cl(3)-Ru(1)-C(35)-C(36)	-90.18(10)
Ru(1)-C(35)-C(36)-C(41)	3.10(17)
Ru(1)-C(35)-C(36)-C(37)	-175.08(10)
C(41)-C(36)-C(37)-C(38)	-0.8(2)
C(35)-C(36)-C(37)-C(38)	177.36(13)
C(36)-C(37)-C(38)-C(39)	-0.1(2)
C(37)-C(38)-C(39)-C(40)	0.9(2)
C(38)-C(39)-C(40)-C(41)	-0.6(2)
C(39)-C(40)-C(41)-O(42)	-178.94(13)
C(39)-C(40)-C(41)-C(36)	-0.4(2)
C(37)-C(36)-C(41)-O(42)	179.80(12)
C(35)-C(36)-C(41)-O(42)	1.54(18)
C(37)-C(36)-C(41)-C(40)	1.1(2)
C(35)-C(36)-C(41)-C(40)	-177.18(13)
C(40)-C(41)-O(42)-C(43)	-15.4(2)
C(36)-C(41)-O(42)-C(43)	165.97(12)
C(40)-C(41)-O(42)-Ru(1)	174.21(12)
C(36)-C(41)-O(42)-Ru(1)	-4.45(14)
C(35)-Ru(1)-O(42)-C(41)	4.88(9)
C(1)-Ru(1)-O(42)-C(41)	-114.0(11)
Cl(2)-Ru(1)-O(42)-C(41)	-95.20(8)
Cl(3)-Ru(1)-O(42)-C(41)	105.23(8)
C(35)-Ru(1)-O(42)-C(43)	-164.29(12)

C(1)-Ru(1)-O(42)-C(43)	76.8(12)
Cl(2)-Ru(1)-O(42)-C(43)	95.63(11)
Cl(3)-Ru(1)-O(42)-C(43)	-63.95(11)
C(41)-O(42)-C(43)-C(44)	168.28(12)
Ru(1)-O(42)-C(43)-C(44)	-23.36(16)
C(41)-O(42)-C(43)-C(45)	-68.94(15)
Ru(1)-O(42)-C(43)-C(45)	99.42(12)
C(63)-O(60)-C(61)-C(62)	179.3(18)
C(61)-O(60)-C(63)-C(64)	-166(2)

Figure S2. ORTEP plot for 1,3-(2,6-dimethylphenyl)-4,5-imidazolin-2-ylidene ruthenium isopropoxybenzylidene dichloride **4**

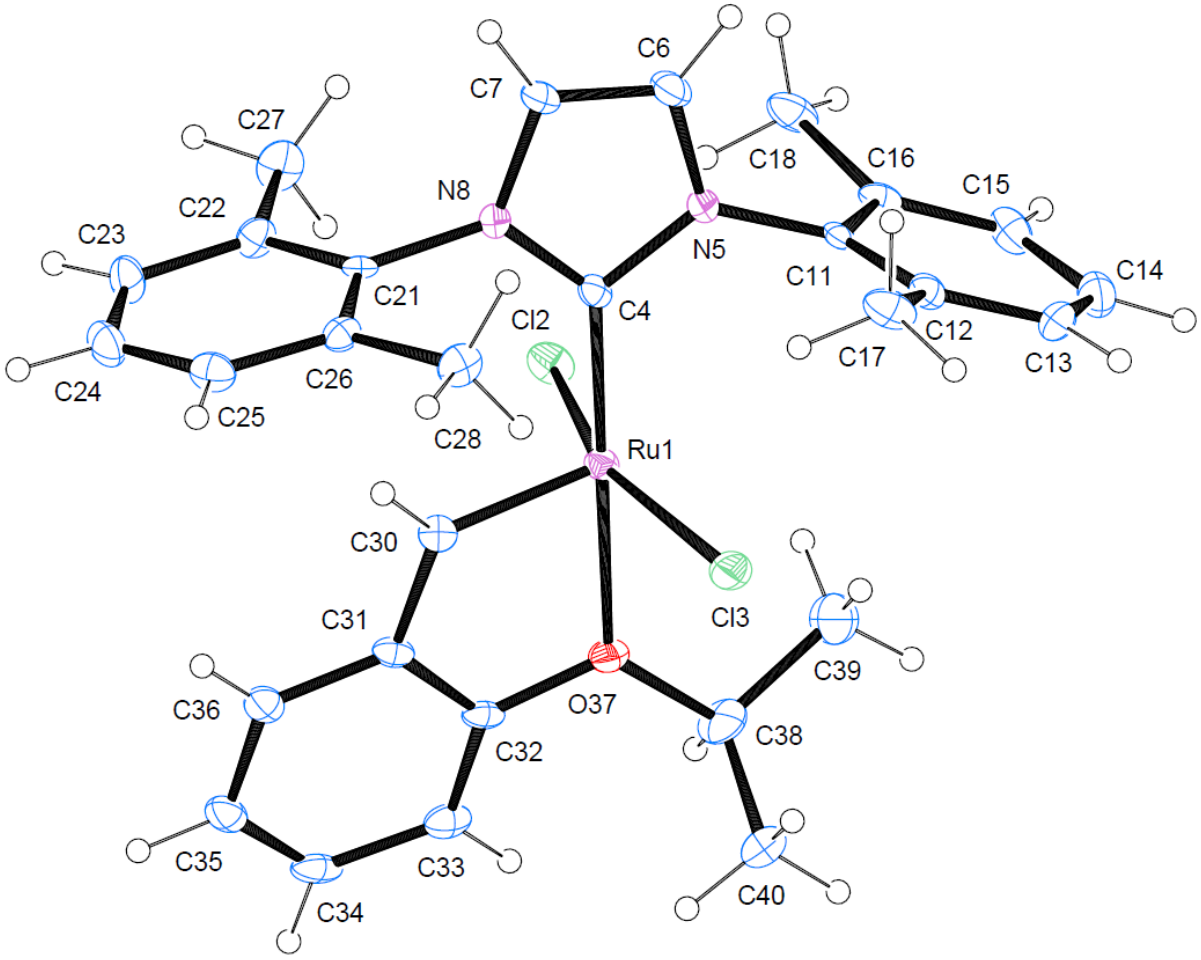

Table S8. Crystal data and structure refinement for **4**.

Identification code	cc06evy1n	
Empirical formula	$3(C_{29}H_{32}Cl_2N_2ORu)$, 1/4(O)	
Formula weight	1790.66	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 17.0768(6) Å	α= 108.116(3)°
	b = 17.4168(6) Å	β= 97.210(3)°
	c = 17.9705(6) Å	γ = 119.219(2)°
Volume	4178.5(2) $Å^3$	
Z	2	
Density (calculated)	1.429 Mg/m^3	
Absorption coefficient	0.779 mm^{-1}	
F(000)	1840	
Crystal size	0.27 x 0.07 x 0.02 mm^3	
Theta range for data collection	1.38 to 27.48°	
Index ranges	-22<=h<=21, -22<=k<=21, 0<=l<=23	
Reflections collected	105659	
Independent reflections	19099 [R(int) = 0.1310]	
Completeness to theta = 27.48°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9281 and 0.8243	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19099 / 360 / 1043	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.0919	
R indices (all data)	R1 = 0.1415, wR2 = 0.1169	
Largest diff. peak and hole	1.161 and -0.767 $e.Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	976(1)	3222(1)	6064(1)	20(1)
Cl(2)	701(1)	2118(1)	6639(1)	30(1)
Cl(3)	1405(1)	3961(1)	5171(1)	32(1)
C(4)	-401(3)	2633(3)	5563(3)	20(1)
N(5)	-954(3)	1846(3)	4799(2)	22(1)
C(6)	-1896(4)	1545(3)	4610(3)	29(1)
C(7)	-1962(4)	2123(3)	5256(3)	32(1)
N(8)	-1049(3)	2786(3)	5836(2)	21(1)
C(11)	-608(3)	1432(3)	4212(3)	19(1)
C(12)	-389(4)	1776(3)	3618(3)	24(1)
C(13)	-44(4)	1374(4)	3061(3)	31(1)
C(14)	59(4)	656(4)	3099(3)	34(2)
C(15)	-223(4)	272(4)	3657(3)	32(1)
C(16)	-579(3)	647(3)	4218(3)	24(1)
C(17)	-586(4)	2494(3)	3514(3)	34(1)
C(18)	-1011(4)	156(3)	4747(3)	35(2)
C(21)	-857(3)	3582(3)	6579(3)	21(1)
C(22)	-920(4)	3454(3)	7292(3)	26(1)
C(23)	-768(4)	4226(4)	7979(3)	32(1)
C(24)	-591(4)	5063(4)	7928(3)	34(2)
C(25)	-535(4)	5176(4)	7202(3)	30(1)
C(26)	-667(3)	4429(3)	6513(3)	22(1)
C(27)	-1123(4)	2527(4)	7338(3)	35(2)
C(28)	-594(4)	4535(4)	5719(3)	30(1)
C(30)	1293(3)	4269(3)	6984(3)	21(1)
C(31)	2226(3)	4813(3)	7606(3)	21(1)
C(32)	2871(3)	4565(3)	7434(3)	22(1)
C(33)	3737(4)	4990(4)	8001(3)	28(1)
C(34)	3980(4)	5712(4)	8771(3)	32(1)
C(35)	3391(4)	6008(3)	8960(3)	30(1)
C(36)	2503(4)	5557(3)	8376(3)	26(1)
O(37)	2519(2)	3841(2)	6642(2)	28(1)
C(38)	3145(4)	3613(4)	6293(4)	41(2)
C(39)	2518(4)	2658(4)	5525(4)	59(2)

C(40)	3846(4)	4443(4)	6109(4)	50(2)
Ru(41)	2305(1)	3476(1)	1370(1)	19(1)
Cl(42)	660(1)	2653(1)	1045(1)	28(1)
Cl(43)	3803(1)	3726(1)	1726(1)	34(1)
C(44)	2256(3)	3342(3)	221(3)	20(1)
N(45)	2004(3)	2505(3)	-440(2)	18(1)
C(46)	1969(4)	2611(3)	-1170(3)	26(1)
C(47)	2220(4)	3525(3)	-989(3)	26(1)
N(48)	2387(3)	3956(3)	-147(2)	22(1)
C(51)	1817(4)	1611(3)	-418(3)	20(1)
C(52)	2574(4)	1507(3)	-265(3)	22(1)
C(53)	2369(4)	621(3)	-289(3)	26(1)
C(54)	1449(4)	-130(4)	-475(3)	29(1)
C(55)	706(4)	-27(3)	-655(3)	28(1)
C(56)	869(4)	838(3)	-643(3)	21(1)
C(57)	3574(3)	2285(3)	-144(3)	32(1)
C(58)	53(3)	919(3)	-917(3)	30(1)
C(61A)[a]	2813(7)	4991(6)	286(8)	26(2)
C(62A)[a]	2204(8)	5300(6)	304(6)	33(2)
C(63A)[a]	2611(9)	6302(6)	742(8)	45(2)
C(64A)[a]	3602(9)	6937(7)	1134(8)	49(2)
C(65A)[a]	4179(8)	6604(6)	1099(5)	48(2)
C(66A)[a]	3821(8)	5614(7)	667(7)	34(2)
C(67A)[a]	1154(7)	4578(8)	-114(7)	43(3)
C(68A)[a]	4437(6)	5246(6)	599(5)	38(2)
C(61B)[b]	2441(12)	4895(12)	201(17)	35(3)
C(62B)[b]	1627(15)	4898(12)	61(14)	37(3)
C(63B)[b]	1766(13)	5812(10)	366(10)	40(3)
C(64B)[b]	2690(14)	6644(11)	840(15)	45(3)
C(65B)[b]	3451(17)	6596(12)	977(16)	49(3)
C(66B)[b]	3378(13)	5709(10)	627(11)	40(3)
C(67B)[b]	670(12)	3963(12)	-425(10)	35(4)
C(68B)[b]	4210(13)	5664(17)	801(16)	47(5)
C(70)	2631(4)	4723(3)	1876(3)	30(1)
C(71)	2747(4)	5144(3)	2740(3)	25(1)
C(72)	2579(4)	4565(3)	3159(3)	23(1)
C(73)	2640(3)	4915(4)	3993(3)	26(1)
C(74)	2894(4)	5865(4)	4390(3)	30(1)
C(75)	3096(4)	6463(4)	3992(3)	31(1)

C(76)	3001(4)	6095(3)	3164(3)	30(1)
O(77)	2357(2)	3653(2)	2688(2)	22(1)
C(78)	2358(4)	3043(3)	3086(3)	24(1)
C(79)	1976(4)	2066(3)	2390(3)	31(1)
C(80)	3352(4)	3498(4)	3657(3)	40(2)
Ru(81)	5121(1)	403(1)	2687(1)	18(1)
Cl(82)	5869(1)	1396(1)	4105(1)	25(1)
Cl(83)	3862(1)	-844(1)	1485(1)	37(1)
C(84)	5053(4)	1430(3)	2483(3)	23(1)
N(85)	4380(3)	1620(3)	2636(2)	24(1)
C(86)	4494(4)	2377(4)	2454(3)	33(1)
C(87)	5251(4)	2683(4)	2196(3)	39(2)
N(88)	5584(3)	2108(3)	2216(2)	24(1)
C(91)	3625(4)	1099(3)	2924(3)	24(1)
C(92)	2749(4)	294(4)	2336(3)	28(1)
C(93)	2037(4)	-220(4)	2615(4)	36(2)
C(94)	2172(4)	76(4)	3453(4)	39(2)
C(95)	3009(4)	900(4)	4014(4)	36(2)
C(96)	3762(4)	1442(4)	3769(3)	29(1)
C(97)	2545(4)	29(4)	1418(3)	38(2)
C(98)	4642(4)	2398(4)	4393(3)	39(2)
C(101)	6370(4)	2228(3)	1933(3)	22(1)
C(102)	7293(4)	2833(3)	2518(3)	24(1)
C(103)	8023(4)	2920(4)	2210(3)	31(1)
C(104)	7861(4)	2439(4)	1385(4)	35(1)
C(105)	6946(4)	1867(4)	821(3)	31(1)
C(106)	6175(4)	1747(3)	1086(3)	25(1)
C(107)	7469(4)	3363(4)	3419(3)	38(2)
C(108)	5178(4)	1160(4)	487(3)	32(1)
C(110)	6114(3)	499(3)	2340(3)	21(1)
C(111)	6433(3)	-110(3)	2428(3)	19(1)
C(112)	5960(3)	-767(3)	2755(3)	19(1)
C(113)	6242(4)	-1359(4)	2863(3)	26(1)
C(114)	7030(4)	-1273(4)	2643(3)	29(1)
C(115)	7505(4)	-639(4)	2317(3)	28(1)
C(116)	7206(4)	-63(3)	2200(3)	26(1)
O(117)	5210(2)	-749(2)	2944(2)	19(1)
C(118)	4745(4)	-1270(4)	3429(3)	29(1)
C(119)	3837(4)	-1295(4)	3358(3)	32(1)

C(120)	5397(4)	-780(4)	4312(3)	38(2)
O(1W)[c]	5058(10)	3729(10)	6957(9)	37(4)

a) Occupation parameter: 0.655(6)

b) Occupation parameter: 0.345(6)

c) Occupation parameter: 0.25 (Not refined)

Table S10. Bond lengths [Å] for **4**

Ru(1)-C(30)	1.813(4)
Ru(1)-C(4)	1.982(5)
Ru(1)-O(37)	2.243(3)
Ru(1)-Cl(3)	2.3297(14)
Ru(1)-Cl(2)	2.3374(13)
C(4)-N(8)	1.370(6)
C(4)-N(5)	1.376(5)
N(5)-C(6)	1.380(6)
N(5)-C(11)	1.443(6)
C(6)-C(7)	1.339(6)
C(6)-H(6)	0.9500
C(7)-N(8)	1.391(6)
C(7)-H(7)	0.9500
N(8)-C(21)	1.453(5)
C(11)-C(12)	1.385(6)
C(11)-C(16)	1.396(6)
C(12)-C(13)	1.396(7)
C(12)-C(17)	1.502(7)
C(13)-C(14)	1.364(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.383(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.394(7)
C(15)-H(15)	0.9500
C(16)-C(18)	1.498(7)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(21)-C(22)	1.375(7)
C(21)-C(26)	1.396(6)
C(22)-C(23)	1.393(6)
C(22)-C(27)	1.510(6)
C(23)-C(24)	1.373(7)
C(23)-H(23)	0.9500

C(24)-C(25)	1.386(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.385(6)
C(25)-H(25)	0.9500
C(26)-C(28)	1.508(7)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(30)-C(31)	1.452(6)
C(30)-H(30)	0.9500
C(31)-C(36)	1.392(6)
C(31)-C(32)	1.400(7)
C(32)-C(33)	1.364(7)
C(32)-O(37)	1.380(5)
C(33)-C(34)	1.390(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.369(7)
C(34)-H(34)	0.9500
C(35)-C(36)	1.395(7)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
O(37)-C(38)	1.457(6)
C(38)-C(39)	1.510(7)
C(38)-C(40)	1.528(8)
C(38)-H(38)	1.0000
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
Ru(41)-C(70)	1.822(4)
Ru(41)-C(44)	1.991(5)
Ru(41)-O(77)	2.274(3)
Ru(41)-Cl(42)	2.3289(14)
Ru(41)-Cl(43)	2.3389(14)

C(44)-N(48)	1.368(6)
C(44)-N(45)	1.380(5)
N(45)-C(46)	1.378(6)
N(45)-C(51)	1.442(6)
C(46)-C(47)	1.342(6)
C(46)-H(46)	0.9500
C(47)-N(48)	1.382(6)
C(47)-H(47)	0.9500
N(48)-C(61A)	1.447(9)
N(48)-C(61B)	1.510(18)
C(51)-C(52)	1.397(7)
C(51)-C(56)	1.402(6)
C(52)-C(53)	1.391(6)
C(52)-C(57)	1.504(7)
C(53)-C(54)	1.372(7)
C(53)-H(53)	0.9500
C(54)-C(55)	1.377(7)
C(54)-H(54)	0.9500
C(55)-C(56)	1.385(6)
C(55)-H(55)	0.9500
C(56)-C(58)	1.505(7)
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(61A)-C(62A)	1.383(12)
C(61A)-C(66A)	1.424(13)
C(62A)-C(63A)	1.404(11)
C(62A)-C(67A)	1.495(12)
C(63A)-C(64A)	1.405(18)
C(63A)-H(63A)	0.9500
C(64A)-C(65A)	1.363(17)
C(64A)-H(64A)	0.9500
C(65A)-C(66A)	1.404(12)
C(65A)-H(65A)	0.9500
C(66A)-C(68A)	1.474(14)
C(67A)-H(67A)	0.9800

C(67A)-H(67B)	0.9800
C(67A)-H(67C)	0.9800
C(68A)-H(68A)	0.9800
C(68A)-H(68B)	0.9800
C(68A)-H(68C)	0.9800
C(61B)-C(62B)	1.384(17)
C(61B)-C(66B)	1.400(17)
C(62B)-C(63B)	1.395(16)
C(62B)-C(67B)	1.499(18)
C(63B)-C(64B)	1.41(2)
C(63B)-H(63B)	0.9500
C(64B)-C(65B)	1.34(3)
C(64B)-H(64B)	0.9500
C(65B)-C(66B)	1.409(17)
C(65B)-H(65B)	0.9500
C(66B)-C(68B)	1.462(19)
C(67B)-H(67D)	0.9800
C(67B)-H(67E)	0.9800
C(67B)-H(67F)	0.9800
C(68B)-H(68D)	0.9800
C(68B)-H(68E)	0.9800
C(68B)-H(68F)	0.9800
C(70)-C(71)	1.435(6)
C(70)-H(70)	0.9500
C(71)-C(72)	1.383(7)
C(71)-C(76)	1.394(6)
C(72)-O(77)	1.370(5)
C(72)-C(73)	1.400(6)
C(73)-C(74)	1.387(6)
C(73)-H(73)	0.9500
C(74)-C(75)	1.374(7)
C(74)-H(74)	0.9500
C(75)-C(76)	1.377(7)
C(75)-H(75)	0.9500
C(76)-H(76)	0.9500
O(77)-C(78)	1.454(5)
C(78)-C(79)	1.508(6)
C(78)-C(80)	1.519(7)
C(78)-H(78)	1.0000

C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800
Ru(81)-C(110)	1.829(5)
Ru(81)-C(84)	1.986(5)
Ru(81)-O(117)	2.263(3)
Ru(81)-Cl(83)	2.3156(13)
Ru(81)-Cl(82)	2.3237(12)
C(84)-N(88)	1.365(6)
C(84)-N(85)	1.378(6)
N(85)-C(86)	1.383(6)
N(85)-C(91)	1.440(6)
C(86)-C(87)	1.342(7)
C(86)-H(86)	0.9500
C(87)-N(88)	1.379(6)
C(87)-H(87)	0.9500
N(88)-C(101)	1.437(6)
C(91)-C(96)	1.388(7)
C(91)-C(92)	1.398(7)
C(92)-C(93)	1.379(7)
C(92)-C(97)	1.511(7)
C(93)-C(94)	1.379(7)
C(93)-H(93)	0.9500
C(94)-C(95)	1.361(8)
C(94)-H(94)	0.9500
C(95)-C(96)	1.397(7)
C(95)-H(95)	0.9500
C(96)-C(98)	1.505(7)
C(97)-H(97A)	0.9800
C(97)-H(97B)	0.9800
C(97)-H(97C)	0.9800
C(98)-H(98A)	0.9800
C(98)-H(98B)	0.9800
C(98)-H(98C)	0.9800
C(101)-C(106)	1.392(6)
C(101)-C(102)	1.405(7)

C(102)-C(103)	1.388(7)
C(102)-C(107)	1.497(6)
C(103)-C(104)	1.369(7)
C(103)-H(103)	0.9500
C(104)-C(105)	1.384(7)
C(104)-H(104)	0.9500
C(105)-C(106)	1.398(7)
C(105)-H(105)	0.9500
C(106)-C(108)	1.503(7)
C(107)-H(10A)	0.9800
C(107)-H(10B)	0.9800
C(107)-H(10C)	0.9800
C(108)-H(10D)	0.9800
C(108)-H(10E)	0.9800
C(108)-H(10F)	0.9800
C(110)-C(111)	1.447(6)
C(110)-H(110)	0.9500
C(111)-C(112)	1.393(6)
C(111)-C(116)	1.403(7)
C(112)-O(117)	1.378(5)
C(112)-C(113)	1.385(6)
C(113)-C(114)	1.401(7)
C(113)-H(113)	0.9500
C(114)-C(115)	1.366(7)
C(114)-H(114)	0.9500
C(115)-C(116)	1.385(7)
C(115)-H(115)	0.9500
C(116)-H(116)	0.9500
O(117)-C(118)	1.475(6)
C(118)-C(120)	1.508(7)
C(118)-C(119)	1.517(7)
C(118)-H(118)	1.0000
C(119)-H(11A)	0.9800
C(119)-H(11B)	0.9800
C(119)-H(11C)	0.9800
C(120)-H(12A)	0.9800
C(120)-H(12B)	0.9800
C(120)-H(12C)	0.9800

Table S11. Angles [°] for **4**.

C(30)-Ru(1)-C(4)	100.9(2)
C(30)-Ru(1)-O(37)	79.82(18)
C(4)-Ru(1)-O(37)	177.84(16)
C(30)-Ru(1)-Cl(3)	99.53(15)
C(4)-Ru(1)-Cl(3)	93.69(14)
O(37)-Ru(1)-Cl(3)	88.16(10)
C(30)-Ru(1)-Cl(2)	99.45(15)
C(4)-Ru(1)-Cl(2)	93.14(14)
O(37)-Ru(1)-Cl(2)	84.73(9)
Cl(3)-Ru(1)-Cl(2)	158.20(5)
N(8)-C(4)-N(5)	102.9(4)
N(8)-C(4)-Ru(1)	134.0(3)
N(5)-C(4)-Ru(1)	123.0(3)
C(4)-N(5)-C(6)	111.7(4)
C(4)-N(5)-C(11)	125.7(4)
C(6)-N(5)-C(11)	122.3(4)
C(7)-C(6)-N(5)	107.1(4)
C(7)-C(6)-H(6)	126.4
N(5)-C(6)-H(6)	126.4
C(6)-C(7)-N(8)	106.8(5)
C(6)-C(7)-H(7)	126.6
N(8)-C(7)-H(7)	126.6
C(4)-N(8)-C(7)	111.6(4)
C(4)-N(8)-C(21)	127.5(4)
C(7)-N(8)-C(21)	120.6(4)
C(12)-C(11)-C(16)	122.0(4)
C(12)-C(11)-N(5)	118.8(4)
C(16)-C(11)-N(5)	119.0(4)
C(11)-C(12)-C(13)	117.9(5)
C(11)-C(12)-C(17)	122.0(5)
C(13)-C(12)-C(17)	119.9(5)
C(14)-C(13)-C(12)	120.7(5)
C(14)-C(13)-H(13)	119.6
C(12)-C(13)-H(13)	119.6
C(13)-C(14)-C(15)	121.0(5)
C(13)-C(14)-H(14)	119.5
C(15)-C(14)-H(14)	119.5

C(14)-C(15)-C(16)	120.0(5)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(15)-C(16)-C(11)	118.0(5)
C(15)-C(16)-C(18)	120.8(5)
C(11)-C(16)-C(18)	120.9(5)
C(12)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(22)-C(21)-C(26)	123.2(4)
C(22)-C(21)-N(8)	119.5(4)
C(26)-C(21)-N(8)	117.2(4)
C(21)-C(22)-C(23)	117.3(5)
C(21)-C(22)-C(27)	121.5(4)
C(23)-C(22)-C(27)	121.2(5)
C(24)-C(23)-C(22)	120.7(5)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	121.2(5)
C(23)-C(24)-H(24)	119.4
C(25)-C(24)-H(24)	119.4
C(26)-C(25)-C(24)	119.5(5)
C(26)-C(25)-H(25)	120.2
C(24)-C(25)-H(25)	120.2
C(25)-C(26)-C(21)	118.1(5)
C(25)-C(26)-C(28)	120.9(5)
C(21)-C(26)-C(28)	121.0(4)
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5

C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(31)-C(30)-Ru(1)	118.1(4)
C(31)-C(30)-H(30)	120.9
Ru(1)-C(30)-H(30)	120.9
C(36)-C(31)-C(32)	118.4(5)
C(36)-C(31)-C(30)	122.9(5)
C(32)-C(31)-C(30)	118.7(4)
C(33)-C(32)-O(37)	124.9(5)
C(33)-C(32)-C(31)	122.7(5)
O(37)-C(32)-C(31)	112.4(4)
C(32)-C(33)-C(34)	117.2(5)
C(32)-C(33)-H(33)	121.4
C(34)-C(33)-H(33)	121.4
C(35)-C(34)-C(33)	122.4(5)
C(35)-C(34)-H(34)	118.8
C(33)-C(34)-H(34)	118.8
C(34)-C(35)-C(36)	119.6(5)
C(34)-C(35)-H(35)	120.2
C(36)-C(35)-H(35)	120.2
C(31)-C(36)-C(35)	119.6(5)
C(31)-C(36)-H(36)	120.2
C(35)-C(36)-H(36)	120.2
C(32)-O(37)-C(38)	120.3(4)
C(32)-O(37)-Ru(1)	109.8(3)
C(38)-O(37)-Ru(1)	129.8(3)
O(37)-C(38)-C(39)	107.1(4)
O(37)-C(38)-C(40)	110.3(4)
C(39)-C(38)-C(40)	112.7(5)
O(37)-C(38)-H(38)	108.9
C(39)-C(38)-H(38)	108.9
C(40)-C(38)-H(38)	108.9

C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(70)-Ru(41)-C(44)	100.5(2)
C(70)-Ru(41)-O(77)	78.39(18)
C(44)-Ru(41)-O(77)	178.83(16)
C(70)-Ru(41)-Cl(42)	99.19(17)
C(44)-Ru(41)-Cl(42)	93.68(14)
O(77)-Ru(41)-Cl(42)	86.08(9)
C(70)-Ru(41)-Cl(43)	100.40(18)
C(44)-Ru(41)-Cl(43)	94.08(14)
O(77)-Ru(41)-Cl(43)	86.56(9)
Cl(42)-Ru(41)-Cl(43)	157.20(5)
N(48)-C(44)-N(45)	102.0(4)
N(48)-C(44)-Ru(41)	133.0(3)
N(45)-C(44)-Ru(41)	124.9(3)
C(46)-N(45)-C(44)	111.8(4)
C(46)-N(45)-C(51)	121.0(4)
C(44)-N(45)-C(51)	127.2(4)
C(47)-C(46)-N(45)	107.4(4)
C(47)-C(46)-H(46)	126.3
N(45)-C(46)-H(46)	126.3
C(46)-C(47)-N(48)	106.0(4)
C(46)-C(47)-H(47)	127.0
N(48)-C(47)-H(47)	127.0
C(44)-N(48)-C(47)	112.8(4)
C(44)-N(48)-C(61A)	125.6(6)
C(47)-N(48)-C(61A)	120.8(7)
C(44)-N(48)-C(61B)	127.1(12)
C(47)-N(48)-C(61B)	118.1(12)

C(61A)-N(48)-C(61B)	21.5(6)
C(52)-C(51)-C(56)	122.0(4)
C(52)-C(51)-N(45)	118.9(4)
C(56)-C(51)-N(45)	118.7(4)
C(53)-C(52)-C(51)	117.8(5)
C(53)-C(52)-C(57)	119.7(5)
C(51)-C(52)-C(57)	122.3(4)
C(54)-C(53)-C(52)	120.7(5)
C(54)-C(53)-H(53)	119.6
C(52)-C(53)-H(53)	119.6
C(53)-C(54)-C(55)	120.7(5)
C(53)-C(54)-H(54)	119.6
C(55)-C(54)-H(54)	119.6
C(54)-C(55)-C(56)	121.0(5)
C(54)-C(55)-H(55)	119.5
C(56)-C(55)-H(55)	119.5
C(55)-C(56)-C(51)	117.5(5)
C(55)-C(56)-C(58)	120.9(5)
C(51)-C(56)-C(58)	121.4(4)
C(52)-C(57)-H(57A)	109.5
C(52)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(52)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(56)-C(58)-H(58A)	109.5
C(56)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(56)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(62A)-C(61A)-C(66A)	125.0(8)
C(62A)-C(61A)-N(48)	117.2(8)
C(66A)-C(61A)-N(48)	117.8(8)
C(61A)-C(62A)-C(63A)	117.5(10)
C(61A)-C(62A)-C(67A)	120.3(8)
C(63A)-C(62A)-C(67A)	122.3(10)
C(62A)-C(63A)-C(64A)	119.2(11)
C(62A)-C(63A)-H(63A)	120.4

C(64A)-C(63A)-H(63A)	120.4
C(65A)-C(64A)-C(63A)	121.6(9)
C(65A)-C(64A)-H(64A)	119.2
C(63A)-C(64A)-H(64A)	119.2
C(64A)-C(65A)-C(66A)	122.2(10)
C(64A)-C(65A)-H(65A)	118.9
C(66A)-C(65A)-H(65A)	118.9
C(65A)-C(66A)-C(61A)	114.5(11)
C(65A)-C(66A)-C(68A)	122.9(10)
C(61A)-C(66A)-C(68A)	122.5(8)
C(62B)-C(61B)-C(66B)	126.7(16)
C(62B)-C(61B)-N(48)	120.9(13)
C(66B)-C(61B)-N(48)	112.4(13)
C(61B)-C(62B)-C(63B)	116.0(17)
C(61B)-C(62B)-C(67B)	120.5(14)
C(63B)-C(62B)-C(67B)	123.4(16)
C(62B)-C(63B)-C(64B)	119.1(16)
C(62B)-C(63B)-H(63B)	120.5
C(64B)-C(63B)-H(63B)	120.5
C(65B)-C(64B)-C(63B)	122.3(15)
C(65B)-C(64B)-H(64B)	118.9
C(63B)-C(64B)-H(64B)	118.9
C(64B)-C(65B)-C(66B)	121.8(19)
C(64B)-C(65B)-H(65B)	119.1
C(66B)-C(65B)-H(65B)	119.1
C(61B)-C(66B)-C(65B)	113.8(16)
C(61B)-C(66B)-C(68B)	124.5(16)
C(65B)-C(66B)-C(68B)	121.2(16)
C(62B)-C(67B)-H(67D)	109.5
C(62B)-C(67B)-H(67E)	109.5
H(67D)-C(67B)-H(67E)	109.5
C(62B)-C(67B)-H(67F)	109.5
H(67D)-C(67B)-H(67F)	109.5
H(67E)-C(67B)-H(67F)	109.5
C(66B)-C(68B)-H(68D)	109.5
C(66B)-C(68B)-H(68E)	109.5
H(68D)-C(68B)-H(68E)	109.5
C(66B)-C(68B)-H(68F)	109.5
H(68D)-C(68B)-H(68F)	109.5

H(68E)-C(68B)-H(68F)	109.5
C(71)-C(70)-Ru(41)	120.3(4)
C(71)-C(70)-H(70)	119.8
Ru(41)-C(70)-H(70)	119.8
C(72)-C(71)-C(76)	119.1(4)
C(72)-C(71)-C(70)	117.7(4)
C(76)-C(71)-C(70)	123.2(5)
O(77)-C(72)-C(71)	114.2(4)
O(77)-C(72)-C(73)	125.0(5)
C(71)-C(72)-C(73)	120.8(4)
C(74)-C(73)-C(72)	118.1(5)
C(74)-C(73)-H(73)	120.9
C(72)-C(73)-H(73)	120.9
C(75)-C(74)-C(73)	121.9(5)
C(75)-C(74)-H(74)	119.0
C(73)-C(74)-H(74)	119.0
C(74)-C(75)-C(76)	119.1(5)
C(74)-C(75)-H(75)	120.4
C(76)-C(75)-H(75)	120.4
C(75)-C(76)-C(71)	120.9(5)
C(75)-C(76)-H(76)	119.6
C(71)-C(76)-H(76)	119.6
C(72)-O(77)-C(78)	119.9(4)
C(72)-O(77)-Ru(41)	109.3(3)
C(78)-O(77)-Ru(41)	129.8(3)
O(77)-C(78)-C(79)	105.9(4)
O(77)-C(78)-C(80)	110.9(4)
C(79)-C(78)-C(80)	112.4(4)
O(77)-C(78)-H(78)	109.2
C(79)-C(78)-H(78)	109.2
C(80)-C(78)-H(78)	109.2
C(78)-C(79)-H(79A)	109.5
C(78)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(78)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(78)-C(80)-H(80A)	109.5
C(78)-C(80)-H(80B)	109.5

H(80A)-C(80)-H(80B)	109.5
C(78)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5
H(80B)-C(80)-H(80C)	109.5
C(110)-Ru(81)-C(84)	101.2(2)
C(110)-Ru(81)-O(117)	79.07(17)
C(84)-Ru(81)-O(117)	178.98(15)
C(110)-Ru(81)-Cl(83)	99.62(14)
C(84)-Ru(81)-Cl(83)	93.33(14)
O(117)-Ru(81)-Cl(83)	87.59(8)
C(110)-Ru(81)-Cl(82)	102.35(14)
C(84)-Ru(81)-Cl(82)	91.63(13)
O(117)-Ru(81)-Cl(82)	87.35(8)
Cl(83)-Ru(81)-Cl(82)	156.06(5)
N(88)-C(84)-N(85)	102.8(4)
N(88)-C(84)-Ru(81)	134.3(4)
N(85)-C(84)-Ru(81)	122.8(4)
C(84)-N(85)-C(86)	111.5(4)
C(84)-N(85)-C(91)	126.0(4)
C(86)-N(85)-C(91)	122.5(4)
C(87)-C(86)-N(85)	106.7(5)
C(87)-C(86)-H(86)	126.7
N(85)-C(86)-H(86)	126.7
C(86)-C(87)-N(88)	107.1(5)
C(86)-C(87)-H(87)	126.4
N(88)-C(87)-H(87)	126.4
C(84)-N(88)-C(87)	111.9(4)
C(84)-N(88)-C(101)	127.6(4)
C(87)-N(88)-C(101)	120.5(4)
C(96)-C(91)-C(92)	121.7(5)
C(96)-C(91)-N(85)	119.6(5)
C(92)-C(91)-N(85)	118.6(5)
C(93)-C(92)-C(91)	118.4(5)
C(93)-C(92)-C(97)	119.7(5)
C(91)-C(92)-C(97)	121.7(5)
C(94)-C(93)-C(92)	120.8(5)
C(94)-C(93)-H(93)	119.6
C(92)-C(93)-H(93)	119.6
C(95)-C(94)-C(93)	119.8(6)

C(95)-C(94)-H(94)	120.1
C(93)-C(94)-H(94)	120.1
C(94)-C(95)-C(96)	121.9(5)
C(94)-C(95)-H(95)	119.0
C(96)-C(95)-H(95)	119.0
C(91)-C(96)-C(95)	117.1(5)
C(91)-C(96)-C(98)	122.0(5)
C(95)-C(96)-C(98)	120.7(5)
C(92)-C(97)-H(97A)	109.5
C(92)-C(97)-H(97B)	109.5
H(97A)-C(97)-H(97B)	109.5
C(92)-C(97)-H(97C)	109.5
H(97A)-C(97)-H(97C)	109.5
H(97B)-C(97)-H(97C)	109.5
C(96)-C(98)-H(98A)	109.5
C(96)-C(98)-H(98B)	109.5
H(98A)-C(98)-H(98B)	109.5
C(96)-C(98)-H(98C)	109.5
H(98A)-C(98)-H(98C)	109.5
H(98B)-C(98)-H(98C)	109.5
C(106)-C(101)-C(102)	123.3(5)
C(106)-C(101)-N(88)	118.0(5)
C(102)-C(101)-N(88)	118.7(4)
C(103)-C(102)-C(101)	116.2(5)
C(103)-C(102)-C(107)	122.5(5)
C(101)-C(102)-C(107)	121.3(5)
C(104)-C(103)-C(102)	122.4(5)
C(104)-C(103)-H(103)	118.8
C(102)-C(103)-H(103)	118.8
C(103)-C(104)-C(105)	120.0(5)
C(103)-C(104)-H(104)	120.0
C(105)-C(104)-H(104)	120.0
C(104)-C(105)-C(106)	120.8(5)
C(104)-C(105)-H(105)	119.6
C(106)-C(105)-H(105)	119.6
C(101)-C(106)-C(105)	117.3(5)
C(101)-C(106)-C(108)	120.6(5)
C(105)-C(106)-C(108)	122.1(5)
C(102)-C(107)-H(10A)	109.5

C(102)-C(107)-H(10B)	109.5
H(10A)-C(107)-H(10B)	109.5
C(102)-C(107)-H(10C)	109.5
H(10A)-C(107)-H(10C)	109.5
H(10B)-C(107)-H(10C)	109.5
C(106)-C(108)-H(10D)	109.5
C(106)-C(108)-H(10E)	109.5
H(10D)-C(108)-H(10E)	109.5
C(106)-C(108)-H(10F)	109.5
H(10D)-C(108)-H(10F)	109.5
H(10E)-C(108)-H(10F)	109.5
C(111)-C(110)-Ru(81)	118.8(4)
C(111)-C(110)-H(110)	120.6
Ru(81)-C(110)-H(110)	120.6
C(112)-C(111)-C(116)	118.4(4)
C(112)-C(111)-C(110)	119.1(5)
C(116)-C(111)-C(110)	122.5(5)
O(117)-C(112)-C(113)	125.8(5)
O(117)-C(112)-C(111)	112.6(4)
C(113)-C(112)-C(111)	121.6(5)
C(112)-C(113)-C(114)	118.1(5)
C(112)-C(113)-H(113)	121.0
C(114)-C(113)-H(113)	121.0
C(115)-C(114)-C(113)	121.7(5)
C(115)-C(114)-H(114)	119.1
C(113)-C(114)-H(114)	119.1
C(114)-C(115)-C(116)	119.5(5)
C(114)-C(115)-H(115)	120.2
C(116)-C(115)-H(115)	120.2
C(115)-C(116)-C(111)	120.7(5)
C(115)-C(116)-H(116)	119.7
C(111)-C(116)-H(116)	119.7
C(112)-O(117)-C(118)	119.2(4)
C(112)-O(117)-Ru(81)	110.3(3)
C(118)-O(117)-Ru(81)	128.9(3)
O(117)-C(118)-C(120)	111.1(4)
O(117)-C(118)-C(119)	105.3(4)
C(120)-C(118)-C(119)	113.5(4)
O(117)-C(118)-H(118)	108.9

C(120)-C(118)-H(118)	108.9
C(119)-C(118)-H(118)	108.9
C(118)-C(119)-H(11A)	109.5
C(118)-C(119)-H(11B)	109.5
H(11A)-C(119)-H(11B)	109.5
C(118)-C(119)-H(11C)	109.5
H(11A)-C(119)-H(11C)	109.5
H(11B)-C(119)-H(11C)	109.5
C(118)-C(120)-H(12A)	109.5
C(118)-C(120)-H(12B)	109.5
H(12A)-C(120)-H(12B)	109.5
C(118)-C(120)-H(12C)	109.5
H(12A)-C(120)-H(12C)	109.5
H(12B)-C(120)-H(12C)	109.5

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	20(1)	17(1)	20(1)	8(1)	6(1)	9(1)
Cl(2)	34(1)	22(1)	32(1)	14(1)	6(1)	14(1)
Cl(3)	31(1)	30(1)	26(1)	15(1)	11(1)	9(1)
C(4)	21(3)	19(2)	14(3)	8(2)	3(2)	8(2)
N(5)	19(3)	22(2)	19(2)	5(2)	5(2)	10(2)
C(6)	21(3)	25(3)	26(3)	2(2)	1(3)	9(3)
C(7)	18(3)	27(3)	28(3)	0(2)	3(3)	6(3)
N(8)	21(3)	22(2)	18(2)	6(2)	7(2)	11(2)
C(11)	15(3)	15(2)	13(3)	3(2)	0(2)	3(2)
C(12)	24(3)	21(3)	19(3)	7(2)	3(2)	10(2)
C(13)	30(3)	33(3)	26(3)	14(3)	15(3)	13(3)
C(14)	31(4)	39(3)	28(3)	5(3)	7(3)	22(3)
C(15)	34(4)	29(3)	29(3)	5(3)	1(3)	22(3)
C(16)	18(3)	19(3)	23(3)	9(2)	-2(2)	5(2)
C(17)	34(4)	23(3)	35(3)	16(3)	1(3)	9(3)
C(18)	36(4)	19(3)	34(3)	11(2)	2(3)	6(3)
C(21)	10(3)	17(2)	23(3)	5(2)	4(2)	2(2)
C(22)	31(3)	27(3)	30(3)	17(2)	15(3)	18(3)
C(23)	40(4)	33(3)	19(3)	10(2)	9(3)	20(3)
C(24)	36(4)	28(3)	31(3)	3(3)	8(3)	20(3)
C(25)	28(3)	24(3)	37(3)	13(3)	8(3)	15(3)
C(26)	20(3)	28(3)	25(3)	14(2)	8(2)	14(2)
C(27)	49(4)	33(3)	40(4)	27(3)	21(3)	26(3)
C(28)	31(3)	36(3)	30(3)	22(3)	11(3)	20(3)
C(30)	22(3)	23(3)	24(3)	13(2)	6(2)	15(2)
C(31)	17(3)	18(2)	25(3)	12(2)	3(2)	7(2)
C(32)	16(3)	20(3)	25(3)	15(2)	4(2)	5(2)
C(33)	22(3)	33(3)	31(3)	23(3)	8(3)	10(3)
C(34)	19(3)	34(3)	28(3)	22(3)	1(3)	0(3)
C(35)	31(4)	20(3)	25(3)	10(2)	7(3)	5(3)
C(36)	29(3)	21(3)	24(3)	12(2)	8(3)	9(3)
O(37)	19(2)	26(2)	32(2)	9(2)	9(2)	10(2)
C(38)	28(4)	44(4)	58(4)	17(3)	21(3)	27(3)
C(39)	47(4)	40(4)	71(5)	0(3)	28(4)	24(3)

C(40)	30(4)	53(4)	47(4)	11(3)	22(3)	14(3)
Ru(41)	23(1)	15(1)	16(1)	7(1)	6(1)	9(1)
Cl(42)	24(1)	26(1)	27(1)	7(1)	7(1)	13(1)
Cl(43)	22(1)	49(1)	27(1)	19(1)	10(1)	15(1)
C(44)	12(3)	17(2)	23(3)	8(2)	3(2)	5(2)
N(45)	20(2)	19(2)	16(2)	9(2)	5(2)	10(2)
C(46)	39(4)	26(3)	15(3)	9(2)	9(3)	18(3)
C(47)	39(4)	28(3)	16(3)	14(2)	13(3)	19(3)
N(48)	29(3)	20(2)	17(2)	10(2)	8(2)	14(2)
C(51)	26(3)	13(2)	22(3)	8(2)	13(2)	11(2)
C(52)	22(3)	23(3)	18(3)	10(2)	8(2)	11(2)
C(53)	25(3)	27(3)	25(3)	10(2)	9(3)	14(3)
C(54)	46(4)	22(3)	24(3)	15(2)	13(3)	20(3)
C(55)	27(3)	20(3)	21(3)	5(2)	6(3)	6(3)
C(56)	26(3)	19(3)	15(3)	5(2)	7(2)	11(2)
C(57)	21(3)	29(3)	36(3)	9(3)	10(3)	11(3)
C(58)	21(3)	24(3)	29(3)	5(2)	5(3)	7(3)
C(61A)	53(4)	20(3)	16(4)	13(3)	16(4)	22(3)
C(62A)	63(4)	24(3)	25(4)	17(3)	23(4)	28(3)
C(63A)	84(4)	25(4)	32(4)	14(4)	30(4)	31(4)
C(64A)	88(5)	22(4)	25(4)	12(4)	24(4)	20(4)
C(65A)	72(5)	25(3)	25(4)	11(3)	14(4)	11(3)
C(66A)	56(5)	24(3)	20(4)	18(3)	8(5)	19(4)
C(67A)	59(6)	46(6)	40(6)	14(5)	16(6)	43(5)
C(68A)	32(5)	33(5)	34(5)	21(4)	6(4)	6(4)
C(61B)	60(5)	21(4)	25(5)	13(4)	20(6)	21(4)
C(62B)	67(6)	27(5)	27(5)	18(5)	23(6)	27(5)
C(63B)	74(5)	30(4)	30(5)	21(4)	29(5)	31(4)
C(64B)	87(5)	18(5)	31(5)	17(5)	30(5)	24(4)
C(65B)	81(5)	22(4)	31(5)	14(5)	25(5)	18(4)
C(66B)	65(5)	23(4)	25(4)	13(4)	19(5)	17(4)
C(67B)	59(8)	40(7)	30(9)	24(7)	18(7)	38(6)
C(68B)	54(7)	29(7)	33(8)	7(7)	20(8)	8(6)
C(70)	47(4)	17(3)	21(3)	11(2)	11(3)	13(3)
C(71)	31(3)	18(3)	19(3)	9(2)	12(2)	8(2)
C(72)	24(3)	22(3)	14(3)	4(2)	6(2)	9(2)
C(73)	24(3)	33(3)	22(3)	14(2)	11(2)	15(3)
C(74)	31(3)	33(3)	16(3)	1(2)	8(3)	18(3)
C(75)	31(3)	21(3)	28(3)	4(2)	4(3)	13(3)

C(76)	38(4)	18(3)	24(3)	8(2)	6(3)	9(3)
O(77)	31(2)	19(2)	17(2)	11(1)	9(2)	14(2)
C(78)	34(3)	29(3)	21(3)	17(2)	13(3)	20(3)
C(79)	40(4)	28(3)	38(3)	23(3)	20(3)	20(3)
C(80)	54(4)	53(4)	33(3)	22(3)	12(3)	41(4)
Ru(81)	21(1)	18(1)	16(1)	8(1)	7(1)	11(1)
Cl(82)	28(1)	27(1)	18(1)	6(1)	5(1)	17(1)
Cl(83)	43(1)	25(1)	26(1)	4(1)	-7(1)	16(1)
C(84)	29(3)	25(3)	16(3)	9(2)	9(2)	15(3)
N(85)	28(3)	24(2)	32(3)	19(2)	17(2)	17(2)
C(86)	46(4)	36(3)	51(4)	37(3)	33(3)	30(3)
C(87)	56(4)	35(3)	51(4)	30(3)	29(3)	33(3)
N(88)	29(3)	21(2)	30(3)	17(2)	14(2)	15(2)
C(91)	29(3)	26(3)	33(3)	21(2)	19(3)	20(3)
C(92)	36(4)	32(3)	34(3)	20(3)	16(3)	27(3)
C(93)	29(4)	33(3)	49(4)	21(3)	10(3)	19(3)
C(94)	38(4)	53(4)	60(4)	41(4)	36(4)	33(4)
C(95)	55(5)	59(4)	39(4)	36(3)	34(3)	49(4)
C(96)	37(4)	41(3)	27(3)	17(3)	13(3)	32(3)
C(97)	41(4)	52(4)	35(3)	20(3)	15(3)	33(3)
C(98)	50(4)	49(4)	36(3)	18(3)	18(3)	39(3)
C(101)	27(3)	21(3)	30(3)	20(2)	17(3)	15(3)
C(102)	31(3)	18(3)	23(3)	14(2)	8(3)	10(3)
C(103)	21(3)	36(3)	36(3)	23(3)	8(3)	12(3)
C(104)	30(4)	40(3)	52(4)	33(3)	24(3)	21(3)
C(105)	43(4)	27(3)	27(3)	13(2)	17(3)	20(3)
C(106)	28(3)	22(3)	25(3)	13(2)	8(3)	13(3)
C(107)	37(4)	29(3)	29(3)	9(3)	3(3)	9(3)
C(108)	36(4)	31(3)	28(3)	12(3)	9(3)	20(3)
C(110)	27(3)	22(3)	20(3)	9(2)	13(2)	16(2)
C(111)	16(3)	14(2)	15(3)	1(2)	-4(2)	5(2)
C(112)	17(3)	23(3)	15(3)	6(2)	6(2)	11(2)
C(113)	32(3)	34(3)	22(3)	19(2)	9(3)	20(3)
C(114)	31(3)	34(3)	28(3)	12(3)	12(3)	23(3)
C(115)	22(3)	33(3)	26(3)	6(2)	9(3)	17(3)
C(116)	29(3)	21(3)	22(3)	7(2)	12(3)	11(3)
O(117)	21(2)	25(2)	21(2)	15(2)	12(2)	15(2)
C(118)	33(4)	33(3)	39(3)	27(3)	23(3)	21(3)
C(119)	33(4)	36(3)	39(3)	26(3)	23(3)	20(3)

C(120)	45(4)	57(4)	35(4)	32(3)	21(3)	35(3)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **4**.

	x	y	z	U(eq)
H(6)	-2402	1024	4114	35
H(7)	-2524	2087	5309	38
H(13)	120	1602	2652	37
H(14)	328	417	2736	41
H(15)	-174	-248	3659	38
H(17A)	-238	2772	3172	51
H(17B)	-378	3017	4061	51
H(17C)	-1270	2163	3243	51
H(18A)	-716	635	5329	53
H(18B)	-903	-360	4687	53
H(18C)	-1697	-129	4569	53
H(23)	-786	4172	8487	38
H(24)	-505	5573	8399	41
H(25)	-407	5761	7178	36
H(27A)	-1664	1964	6851	52
H(27B)	-1274	2514	7844	52
H(27C)	-561	2501	7348	52
H(28A)	-498	5156	5776	44
H(28B)	-1182	3997	5259	44
H(28C)	-54	4520	5604	44
H(30)	860	4456	7057	26
H(33)	4158	4800	7876	34
H(34)	4575	6011	9180	39
H(35)	3586	6517	9487	36
H(36)	2089	5756	8502	32
H(38)	3511	3530	6705	49
H(39A)	2085	2152	5676	88
H(39B)	2916	2472	5279	88
H(39C)	2147	2728	5121	88
H(40A)	3494	4521	5697	75
H(40B)	4276	4290	5891	75
H(40C)	4218	5049	6622	75
H(46)	1799	2126	-1703	31

H(47)	2271	3816	-1364	31
H(53)	2872	535	-175	32
H(54)	1322	-727	-480	35
H(55)	73	-559	-790	34
H(57A)	4024	2324	287	48
H(57B)	3645	2914	27	48
H(57C)	3705	2123	-666	48
H(58A)	-550	301	-1066	45
H(58B)	83	1066	-1401	45
H(58C)	96	1442	-463	45
H(63A)	2221	6547	773	54
H(64A)	3878	7614	1431	59
H(65A)	4845	7058	1377	58
H(67A)	1009	4291	-717	64
H(67B)	826	4906	23	64
H(67C)	937	4063	78	64
H(68A)	5105	5797	823	57
H(68B)	4282	4840	14	57
H(68C)	4333	4857	915	57
H(63B)	1244	5871	255	48
H(64B)	2777	7262	1070	54
H(65B)	4056	7177	1319	58
H(67D)	684	3600	-957	53
H(67E)	189	4106	-526	53
H(67F)	510	3570	-109	53
H(68D)	4790	6324	1050	70
H(68E)	4222	5271	282	70
H(68F)	4175	5366	1188	70
H(70)	2725	5096	1567	37
H(73)	2510	4513	4278	31
H(74)	2930	6110	4954	35
H(75)	3298	7121	4285	37
H(76)	3110	6495	2879	36
H(78)	1919	2964	3417	29
H(79A)	1345	1813	2028	46
H(79B)	1928	1611	2622	46
H(79C)	2408	2139	2066	46
H(80A)	3793	3614	3341	60
H(80B)	3344	3055	3889	60

H(80C)	3560	4117	4109	60
H(86)	4111	2630	2502	40
H(87)	5509	3199	2031	47
H(93)	1445	-784	2225	43
H(94)	1683	-293	3639	47
H(95)	3084	1111	4588	43
H(97A)	2360	433	1280	58
H(97B)	2024	-660	1100	58
H(97C)	3116	143	1277	58
H(98A)	5184	2527	4196	59
H(98B)	4773	2369	4927	59
H(98C)	4544	2922	4464	59
H(103)	8658	3327	2585	37
H(104)	8376	2498	1200	42
H(105)	6841	1553	247	37
H(10A)	7198	2893	3655	57
H(10B)	7169	3726	3477	57
H(10C)	8156	3818	3714	57
H(10D)	4770	612	607	48
H(10E)	5181	912	-82	48
H(10F)	4934	1573	545	48
H(110)	6416	941	2107	25
H(113)	5911	-1810	3081	32
H(114)	7238	-1667	2722	34
H(115)	8038	-594	2173	34
H(116)	7528	369	1964	31
H(118)	4574	-1953	3164	35
H(11A)	3998	-628	3615	47
H(11B)	3472	-1667	3642	47
H(11C)	3454	-1606	2771	47
H(12A)	5957	-808	4315	56
H(12B)	5058	-1116	4629	56
H(12C)	5599	-98	4565	56

Table S14. Torsion angles [°] for **4**.

C(30)-Ru(1)-C(4)-N(8)	-11.3(5)
O(37)-Ru(1)-C(4)-N(8)	99(4)
Cl(3)-Ru(1)-C(4)-N(8)	-111.7(5)
Cl(2)-Ru(1)-C(4)-N(8)	89.0(5)
C(30)-Ru(1)-C(4)-N(5)	174.4(4)
O(37)-Ru(1)-C(4)-N(5)	-75(4)
Cl(3)-Ru(1)-C(4)-N(5)	73.9(4)
Cl(2)-Ru(1)-C(4)-N(5)	-85.4(4)
N(8)-C(4)-N(5)-C(6)	1.0(5)
Ru(1)-C(4)-N(5)-C(6)	176.9(3)
N(8)-C(4)-N(5)-C(11)	174.8(4)
Ru(1)-C(4)-N(5)-C(11)	-9.4(7)
C(4)-N(5)-C(6)-C(7)	-1.1(6)
C(11)-N(5)-C(6)-C(7)	-175.1(5)
N(5)-C(6)-C(7)-N(8)	0.7(6)
N(5)-C(4)-N(8)-C(7)	-0.6(5)
Ru(1)-C(4)-N(8)-C(7)	-175.7(4)
N(5)-C(4)-N(8)-C(21)	-173.9(4)
Ru(1)-C(4)-N(8)-C(21)	10.9(8)
C(6)-C(7)-N(8)-C(4)	0.0(6)
C(6)-C(7)-N(8)-C(21)	173.8(4)
C(4)-N(5)-C(11)-C(12)	-90.9(6)
C(6)-N(5)-C(11)-C(12)	82.2(6)
C(4)-N(5)-C(11)-C(16)	94.3(6)
C(6)-N(5)-C(11)-C(16)	-92.6(6)
C(16)-C(11)-C(12)-C(13)	-6.1(7)
N(5)-C(11)-C(12)-C(13)	179.3(4)
C(16)-C(11)-C(12)-C(17)	168.7(4)
N(5)-C(11)-C(12)-C(17)	-5.8(7)
C(11)-C(12)-C(13)-C(14)	0.9(8)
C(17)-C(12)-C(13)-C(14)	-174.1(5)
C(12)-C(13)-C(14)-C(15)	3.5(8)
C(13)-C(14)-C(15)-C(16)	-2.9(8)
C(14)-C(15)-C(16)-C(11)	-2.2(7)
C(14)-C(15)-C(16)-C(18)	171.5(5)
C(12)-C(11)-C(16)-C(15)	6.7(7)
N(5)-C(11)-C(16)-C(15)	-178.7(4)

C(12)-C(11)-C(16)-C(18)	-166.9(5)
N(5)-C(11)-C(16)-C(18)	7.6(7)
C(4)-N(8)-C(21)-C(22)	-95.9(6)
C(7)-N(8)-C(21)-C(22)	91.3(6)
C(4)-N(8)-C(21)-C(26)	87.8(6)
C(7)-N(8)-C(21)-C(26)	-85.0(6)
C(26)-C(21)-C(22)-C(23)	-1.3(8)
N(8)-C(21)-C(22)-C(23)	-177.5(4)
C(26)-C(21)-C(22)-C(27)	-179.8(5)
N(8)-C(21)-C(22)-C(27)	4.1(7)
C(21)-C(22)-C(23)-C(24)	2.0(8)
C(27)-C(22)-C(23)-C(24)	-179.5(5)
C(22)-C(23)-C(24)-C(25)	-1.7(9)
C(23)-C(24)-C(25)-C(26)	0.5(8)
C(24)-C(25)-C(26)-C(21)	0.2(8)
C(24)-C(25)-C(26)-C(28)	-178.9(5)
C(22)-C(21)-C(26)-C(25)	0.2(8)
N(8)-C(21)-C(26)-C(25)	176.5(4)
C(22)-C(21)-C(26)-C(28)	179.3(5)
N(8)-C(21)-C(26)-C(28)	-4.5(7)
C(4)-Ru(1)-C(30)-C(31)	169.7(4)
O(37)-Ru(1)-C(30)-C(31)	-8.3(4)
Cl(3)-Ru(1)-C(30)-C(31)	-94.6(4)
Cl(2)-Ru(1)-C(30)-C(31)	74.6(4)
Ru(1)-C(30)-C(31)-C(36)	-172.5(4)
Ru(1)-C(30)-C(31)-C(32)	6.1(6)
C(36)-C(31)-C(32)-C(33)	3.2(7)
C(30)-C(31)-C(32)-C(33)	-175.4(5)
C(36)-C(31)-C(32)-O(37)	-178.1(4)
C(30)-C(31)-C(32)-O(37)	3.3(6)
O(37)-C(32)-C(33)-C(34)	179.9(4)
C(31)-C(32)-C(33)-C(34)	-1.6(8)
C(32)-C(33)-C(34)-C(35)	-1.0(8)
C(33)-C(34)-C(35)-C(36)	1.8(8)
C(32)-C(31)-C(36)-C(35)	-2.3(7)
C(30)-C(31)-C(36)-C(35)	176.2(5)
C(34)-C(35)-C(36)-C(31)	-0.1(8)
C(33)-C(32)-O(37)-C(38)	-12.9(7)
C(31)-C(32)-O(37)-C(38)	168.4(4)

C(33)-C(32)-O(37)-Ru(1)	169.6(4)
C(31)-C(32)-O(37)-Ru(1)	-9.0(5)
C(30)-Ru(1)-O(37)-C(32)	9.9(3)
C(4)-Ru(1)-O(37)-C(32)	-101(4)
Cl(3)-Ru(1)-O(37)-C(32)	109.9(3)
Cl(2)-Ru(1)-O(37)-C(32)	-90.7(3)
C(30)-Ru(1)-O(37)-C(38)	-167.2(4)
C(4)-Ru(1)-O(37)-C(38)	82(4)
Cl(3)-Ru(1)-O(37)-C(38)	-67.1(4)
Cl(2)-Ru(1)-O(37)-C(38)	92.2(4)
C(32)-O(37)-C(38)-C(39)	167.0(5)
Ru(1)-O(37)-C(38)-C(39)	-16.2(7)
C(32)-O(37)-C(38)-C(40)	-70.0(6)
Ru(1)-O(37)-C(38)-C(40)	106.8(5)
C(70)-Ru(41)-C(44)-N(48)	-1.9(5)
O(77)-Ru(41)-C(44)-N(48)	20(9)
Cl(42)-Ru(41)-C(44)-N(48)	98.2(5)
Cl(43)-Ru(41)-C(44)-N(48)	-103.3(5)
C(70)-Ru(41)-C(44)-N(45)	-177.7(4)
O(77)-Ru(41)-C(44)-N(45)	-156(8)
Cl(42)-Ru(41)-C(44)-N(45)	-77.6(4)
Cl(43)-Ru(41)-C(44)-N(45)	80.9(4)
N(48)-C(44)-N(45)-C(46)	-1.2(5)
Ru(41)-C(44)-N(45)-C(46)	175.7(3)
N(48)-C(44)-N(45)-C(51)	177.1(4)
Ru(41)-C(44)-N(45)-C(51)	-6.1(7)
C(44)-N(45)-C(46)-C(47)	1.5(6)
C(51)-N(45)-C(46)-C(47)	-176.9(4)
N(45)-C(46)-C(47)-N(48)	-1.0(6)
N(45)-C(44)-N(48)-C(47)	0.5(5)
Ru(41)-C(44)-N(48)-C(47)	-175.9(4)
N(45)-C(44)-N(48)-C(61A)	-169.1(6)
Ru(41)-C(44)-N(48)-C(61A)	14.4(9)
N(45)-C(44)-N(48)-C(61B)	164.1(9)
Ru(41)-C(44)-N(48)-C(61B)	-12.4(11)
C(46)-C(47)-N(48)-C(44)	0.3(6)
C(46)-C(47)-N(48)-C(61A)	170.5(6)
C(46)-C(47)-N(48)-C(61B)	-164.9(9)
C(46)-N(45)-C(51)-C(52)	89.6(6)

C(44)-N(45)-C(51)-C(52)	-88.6(6)
C(46)-N(45)-C(51)-C(56)	-83.4(6)
C(44)-N(45)-C(51)-C(56)	98.5(6)
C(56)-C(51)-C(52)-C(53)	-4.1(7)
N(45)-C(51)-C(52)-C(53)	-176.9(4)
C(56)-C(51)-C(52)-C(57)	171.1(4)
N(45)-C(51)-C(52)-C(57)	-1.6(7)
C(51)-C(52)-C(53)-C(54)	1.4(7)
C(57)-C(52)-C(53)-C(54)	-174.0(5)
C(52)-C(53)-C(54)-C(55)	1.0(8)
C(53)-C(54)-C(55)-C(56)	-0.8(8)
C(54)-C(55)-C(56)-C(51)	-1.8(7)
C(54)-C(55)-C(56)-C(58)	174.3(4)
C(52)-C(51)-C(56)-C(55)	4.3(7)
N(45)-C(51)-C(56)-C(55)	177.0(4)
C(52)-C(51)-C(56)-C(58)	-171.7(4)
N(45)-C(51)-C(56)-C(58)	1.0(7)
C(44)-N(48)-C(61A)-C(62A)	-103.1(10)
C(47)-N(48)-C(61A)-C(62A)	88.0(11)
C(61B)-N(48)-C(61A)-C(62A)	-1(4)
C(44)-N(48)-C(61A)-C(66A)	76.2(13)
C(47)-N(48)-C(61A)-C(66A)	-92.7(12)
C(61B)-N(48)-C(61A)-C(66A)	178(5)
C(66A)-C(61A)-C(62A)-C(63A)	-0.9(18)
N(48)-C(61A)-C(62A)-C(63A)	178.3(10)
C(66A)-C(61A)-C(62A)-C(67A)	-179.5(12)
N(48)-C(61A)-C(62A)-C(67A)	-0.3(15)
C(61A)-C(62A)-C(63A)-C(64A)	0.1(18)
C(67A)-C(62A)-C(63A)-C(64A)	178.7(11)
C(62A)-C(63A)-C(64A)-C(65A)	0(2)
C(63A)-C(64A)-C(65A)-C(66A)	0.5(19)
C(64A)-C(65A)-C(66A)-C(61A)	-1.1(17)
C(64A)-C(65A)-C(66A)-C(68A)	177.9(11)
C(62A)-C(61A)-C(66A)-C(65A)	1.4(19)
N(48)-C(61A)-C(66A)-C(65A)	-177.9(10)
C(62A)-C(61A)-C(66A)-C(68A)	-177.6(11)
N(48)-C(61A)-C(66A)-C(68A)	3.2(19)
C(44)-N(48)-C(61B)-C(62B)	-89(3)
C(47)-N(48)-C(61B)-C(62B)	74(3)

C(61A)-N(48)-C(61B)-C(62B)	177(7)
C(44)-N(48)-C(61B)-C(66B)	93(2)
C(47)-N(48)-C(61B)-C(66B)	-103.7(19)
C(61A)-N(48)-C(61B)-C(66B)	0(3)
C(66B)-C(61B)-C(62B)-C(63B)	1(4)
N(48)-C(61B)-C(62B)-C(63B)	-176(2)
C(66B)-C(61B)-C(62B)-C(67B)	179(2)
N(48)-C(61B)-C(62B)-C(67B)	1(4)
C(61B)-C(62B)-C(63B)-C(64B)	-5(3)
C(67B)-C(62B)-C(63B)-C(64B)	178(2)
C(62B)-C(63B)-C(64B)-C(65B)	3(4)
C(63B)-C(64B)-C(65B)-C(66B)	2(5)
C(62B)-C(61B)-C(66B)-C(65B)	4(4)
N(48)-C(61B)-C(66B)-C(65B)	-179(2)
C(62B)-C(61B)-C(66B)-C(68B)	176(3)
N(48)-C(61B)-C(66B)-C(68B)	-6(3)
C(64B)-C(65B)-C(66B)-C(61B)	-6(4)
C(64B)-C(65B)-C(66B)-C(68B)	-178(3)
C(44)-Ru(41)-C(70)-C(71)	179.8(4)
O(77)-Ru(41)-C(70)-C(71)	0.2(4)
Cl(42)-Ru(41)-C(70)-C(71)	84.2(4)
Cl(43)-Ru(41)-C(70)-C(71)	-84.1(4)
Ru(41)-C(70)-C(71)-C(72)	-1.7(7)
Ru(41)-C(70)-C(71)-C(76)	179.6(4)
C(76)-C(71)-C(72)-O(77)	-178.5(5)
C(70)-C(71)-C(72)-O(77)	2.7(7)
C(76)-C(71)-C(72)-C(73)	1.5(8)
C(70)-C(71)-C(72)-C(73)	-177.3(5)
O(77)-C(72)-C(73)-C(74)	178.6(5)
C(71)-C(72)-C(73)-C(74)	-1.5(8)
C(72)-C(73)-C(74)-C(75)	-0.8(8)
C(73)-C(74)-C(75)-C(76)	3.0(8)
C(74)-C(75)-C(76)-C(71)	-3.0(8)
C(72)-C(71)-C(76)-C(75)	0.8(8)
C(70)-C(71)-C(76)-C(75)	179.5(5)
C(71)-C(72)-O(77)-C(78)	167.2(4)
C(73)-C(72)-O(77)-C(78)	-12.8(7)
C(71)-C(72)-O(77)-Ru(41)	-2.3(5)
C(73)-C(72)-O(77)-Ru(41)	177.7(4)

C(70)-Ru(41)-O(77)-C(72)	1.2(3)
C(44)-Ru(41)-O(77)-C(72)	-21(8)
Cl(42)-Ru(41)-O(77)-C(72)	-99.0(3)
Cl(43)-Ru(41)-O(77)-C(72)	102.5(3)
C(70)-Ru(41)-O(77)-C(78)	-166.9(4)
C(44)-Ru(41)-O(77)-C(78)	171(43)
Cl(42)-Ru(41)-O(77)-C(78)	92.8(4)
Cl(43)-Ru(41)-O(77)-C(78)	-65.6(4)
C(72)-O(77)-C(78)-C(79)	173.5(4)
Ru(41)-O(77)-C(78)-C(79)	-19.4(6)
C(72)-O(77)-C(78)-C(80)	-64.2(6)
Ru(41)-O(77)-C(78)-C(80)	102.8(4)
C(110)-Ru(81)-C(84)-N(88)	-4.0(5)
O(117)-Ru(81)-C(84)-N(88)	102(10)
Cl(83)-Ru(81)-C(84)-N(88)	-104.5(5)
Cl(82)-Ru(81)-C(84)-N(88)	98.9(5)
C(110)-Ru(81)-C(84)-N(85)	178.5(4)
O(117)-Ru(81)-C(84)-N(85)	-76(10)
Cl(83)-Ru(81)-C(84)-N(85)	78.0(4)
Cl(82)-Ru(81)-C(84)-N(85)	-78.6(4)
N(88)-C(84)-N(85)-C(86)	0.9(5)
Ru(81)-C(84)-N(85)-C(86)	179.1(3)
N(88)-C(84)-N(85)-C(91)	179.2(4)
Ru(81)-C(84)-N(85)-C(91)	-2.6(7)
C(84)-N(85)-C(86)-C(87)	-0.9(6)
C(91)-N(85)-C(86)-C(87)	-179.3(5)
N(85)-C(86)-C(87)-N(88)	0.5(6)
N(85)-C(84)-N(88)-C(87)	-0.6(5)
Ru(81)-C(84)-N(88)-C(87)	-178.5(4)
N(85)-C(84)-N(88)-C(101)	-177.1(4)
Ru(81)-C(84)-N(88)-C(101)	5.0(8)
C(86)-C(87)-N(88)-C(84)	0.1(6)
C(86)-C(87)-N(88)-C(101)	176.9(5)
C(84)-N(85)-C(91)-C(96)	93.9(6)
C(86)-N(85)-C(91)-C(96)	-88.0(6)
C(84)-N(85)-C(91)-C(92)	-90.2(6)
C(86)-N(85)-C(91)-C(92)	87.9(6)
C(96)-C(91)-C(92)-C(93)	-6.0(7)
N(85)-C(91)-C(92)-C(93)	178.2(4)

C(96)-C(91)-C(92)-C(97)	168.8(5)
N(85)-C(91)-C(92)-C(97)	-7.0(7)
C(91)-C(92)-C(93)-C(94)	2.4(8)
C(97)-C(92)-C(93)-C(94)	-172.5(5)
C(92)-C(93)-C(94)-C(95)	1.8(8)
C(93)-C(94)-C(95)-C(96)	-2.6(8)
C(92)-C(91)-C(96)-C(95)	5.1(7)
N(85)-C(91)-C(96)-C(95)	-179.1(4)
C(92)-C(91)-C(96)-C(98)	-169.7(5)
N(85)-C(91)-C(96)-C(98)	6.0(7)
C(94)-C(95)-C(96)-C(91)	-0.8(8)
C(94)-C(95)-C(96)-C(98)	174.2(5)
C(84)-N(88)-C(101)-C(106)	92.0(6)
C(87)-N(88)-C(101)-C(106)	-84.3(6)
C(84)-N(88)-C(101)-C(102)	-89.1(6)
C(87)-N(88)-C(101)-C(102)	94.6(6)
C(106)-C(101)-C(102)-C(103)	-1.3(7)
N(88)-C(101)-C(102)-C(103)	179.9(4)
C(106)-C(101)-C(102)-C(107)	177.7(5)
N(88)-C(101)-C(102)-C(107)	-1.1(7)
C(101)-C(102)-C(103)-C(104)	-0.6(7)
C(107)-C(102)-C(103)-C(104)	-179.6(5)
C(102)-C(103)-C(104)-C(105)	2.2(8)
C(103)-C(104)-C(105)-C(106)	-2.0(8)
C(102)-C(101)-C(106)-C(105)	1.4(7)
N(88)-C(101)-C(106)-C(105)	-179.7(4)
C(102)-C(101)-C(106)-C(108)	-176.2(4)
N(88)-C(101)-C(106)-C(108)	2.7(7)
C(104)-C(105)-C(106)-C(101)	0.3(7)
C(104)-C(105)-C(106)-C(108)	177.8(5)
C(84)-Ru(81)-C(110)-C(111)	176.8(3)
O(117)-Ru(81)-C(110)-C(111)	-2.2(3)
Cl(83)-Ru(81)-C(110)-C(111)	-87.8(3)
Cl(82)-Ru(81)-C(110)-C(111)	82.7(3)
Ru(81)-C(110)-C(111)-C(112)	1.5(6)
Ru(81)-C(110)-C(111)-C(116)	-178.1(3)
C(116)-C(111)-C(112)-O(117)	-179.3(4)
C(110)-C(111)-C(112)-O(117)	1.0(6)
C(116)-C(111)-C(112)-C(113)	0.5(7)

C(110)-C(111)-C(112)-C(113)	-179.1(4)
O(117)-C(112)-C(113)-C(114)	-179.5(4)
C(111)-C(112)-C(113)-C(114)	0.7(7)
C(112)-C(113)-C(114)-C(115)	-1.0(7)
C(113)-C(114)-C(115)-C(116)	0.0(7)
C(114)-C(115)-C(116)-C(111)	1.3(7)
C(112)-C(111)-C(116)-C(115)	-1.5(7)
C(110)-C(111)-C(116)-C(115)	178.1(4)
C(113)-C(112)-O(117)-C(118)	10.8(7)
C(111)-C(112)-O(117)-C(118)	-169.3(4)
C(113)-C(112)-O(117)-Ru(81)	177.6(4)
C(111)-C(112)-O(117)-Ru(81)	-2.5(4)
C(110)-Ru(81)-O(117)-C(112)	2.7(3)
C(84)-Ru(81)-O(117)-C(112)	-103(10)
Cl(83)-Ru(81)-O(117)-C(112)	102.9(3)
Cl(82)-Ru(81)-O(117)-C(112)	-100.5(3)
C(110)-Ru(81)-O(117)-C(118)	167.8(4)
C(84)-Ru(81)-O(117)-C(118)	62(10)
Cl(83)-Ru(81)-O(117)-C(118)	-91.9(3)
Cl(82)-Ru(81)-O(117)-C(118)	64.7(3)
C(112)-O(117)-C(118)-C(120)	69.0(5)
Ru(81)-O(117)-C(118)-C(120)	-95.0(4)
C(112)-O(117)-C(118)-C(119)	-167.7(4)
Ru(81)-O(117)-C(118)-C(119)	28.3(5)