Supporting Information

for

A Versatile Precursor for the Synthesis of New Ruthenium Olefin Metathesis Catalysts

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Supporting Information Experimental Section

General Procedures. Manipulation of organometallic compounds was performed using standard Schlenk techniques under an atmosphere of dry argon or in a nitrogen-filled Vacuum Atmospheres drybox ($O_2 < 2$ ppm). NMR spectra were recorded on a Varian Inova (499.85 MHz for ^1H; 202.34 MHz for ^{31}P; 125.69 MHz for ^{13}C) or a Varian Mercury 300 (299.817 for ^1H; 121.39 MHz for ^{31}P; 74.45 MHz for ^{13}C). ^{31}P NMR spectra were referenced using H_3PO_4 ($\delta = 0$ ppm) as an external standard. UV-vis spectra were recorded on an HP 8452A Diode Array Spectrophotometer.

Materials and Methods. Pentane, toluene, benzene, and benzene-d_6 were dried by passage through solvent purification columns.[1] Pyridine was dried by vacuum transfer from CaH_2. All phosphines as well as KTp were obtained from commercial sources and used as received. Ruthenium complex **2** was prepared according to literature procedures.[2,3] Silica gel was obtained from TSI.

$(IMesH_2)(PBn_3)(Cl)_2Ru=CHPh$ (5). Complex **3** (150 mg, 0.21 mmol) and PBn_3 (88 mg, 0.29 mmol) were combined in benzene (10 mL) and stirred for 10 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 4 x 20 mL pentane and dried *in vacuo*. Complex **5** was obtained as a brown-pink powder (130 mg, 73% yield). $^{31}P\{^1H\}$ NMR (C_6D_6): δ 34.7 (s). ^1H NMR (C_6D_6): δ 19.31 (s, 1H, Ru=C*H*Ph), 8.31 (d, 2H, ortho C*H*, J_{HH} = 7 Hz,), 7.36 (7, 1H, para C*H*, J_{HH} = 7.0 Hz), 7.16 (br. s, 19H, $(CH_2Ph)_3P$, meta C*H*, Mes C*H*), 6.64 (s, 2H, Mes C*H*), 3.77 (m, 2H, CH_2CH_2), 3.64 (m, 2H, CH_2CH_2), 3.29 (d, 6H,

benzyl CH_2, J_{HP} = 7.2 Hz), 3.18 (s, 6H, ortho CH_3), 2.78 (s, 6H, ortho CH_3), 2.18 (s, 3H, para CH_3), 2.12 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (C_6D_6): δ 297.50 (m, Ru=*C*HPh), 222.30 (d, Ru-*C*(N)$_2$, J_{CP} = 85 Hz), 151.52, 140.31, 139.54, 137.94, 137.77, 137.30, 135.45, 135.42, 135.39, 131.27, 131.24, 131.21, 130.21, 129.72, 129.00, 126.42, 126.40, 51.72 (d, J_{CP} = 1 Hz), 51.52 (d, J_{CP} = 4 Hz), 25.80, 25.68, 21.36, 21.20, 21.11, 19.13. Anal. Calcd for $C_{49}H_{53}N_2Cl_2PRu$: C, 67.42; H, 6.12; N, 3.21. Found: C, 67.70; H, 6.20; N, 3.26.

(IMesH$_2$)[(*n*-Bu)$_3$P](Cl)$_2$Ru=CHPh (6). Complex **3** (60 mg, 0.083 mmol) and *n*-Bu_3P (24 mg, 0.12 mmol) were combined in benzene (2 mL) and stirred for 10 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 3 mL pentane and dried *in vacuo*. Complex **6** was obtained as a pink powder (45 mg, 70% yield). $^{31}P\{^1H\}$ NMR (C_6D_6): δ 20.4 (s). ^1H NMR (C_6D_6): δ 19.45 (s, 1H, Ru=C*H*Ph), 8.25 (d, 2H, ortho C*H*, J_{HH} = 8 Hz), 7.20-6.94 (multiple peaks, 5H, para C*H*, meta C*H*, and Mes C*H*), 6.29 (s, 2H, Mes C*H*), 3.34 (m, 4H, CH_2CH_2), 2.83 (s, 6H, ortho CH_3), 2.42 (s, 6H, ortho CH_3), 2.23 (s, 3H, para CH_3), 1.87 (s, 3H, para CH_3), 1.62-0.74 (multiple peaks, 27H, *n*-Bu_3P). $^{13}C\{^1H\}$ NMR (C_6D_6): δ 295.96 (m, Ru=*C*HPh), 223.22 (d, Ru-*C*(N)$_2$, J_{CP} = 82 Hz), 151.87 (d, J_{CP} = 2 Hz), 139.84, 138.49, 138.14, 137.78, 137.37, 135.78, 131.56, 130.47, 130.16, 129.70, 128.76, 128.67, 52.13 (d, J_{CP} = 4 Hz), 51.38 (d, J_{CP} = 2 Hz), 25.60, 25.01, 21.59, 21.36, 21.18, 20.99, 19.17, 14.00. Anal. Calcd for $C_{49}H_{59}N_2Cl_2PRu$: C, 62.32; H, 7.71; N, 3.637. Found: C, 62.55; H, 7.84; N, 3.66.

(IMesH$_2$)[(*p*-CF$_3$C$_6$H$_4$)$_3$P](Cl)$_2$Ru=CHPh (7). Complex **3** (120 mg, 0.17 mmol) and (*p*-$CF_3C_6H_4)_3P$ (81 mg, 0.18 mmol) were combined in benzene (5 mL), and the resulting solution was stirred for 20 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 10 mL pentane. The pink solid residue was dried under vacuum to afford 40 mg of product. The pentane washes were then concentrated under vacuum and purified by column chromatography on silica gel (solvent system of pentane/diethyl ether 5:1). A combined yield of 90 mg (53% yield) of the light pink product was obtained over the two purification steps. $^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ 40.20 (s). ^{19}F NMR (CD_2Cl_2): δ –63.17 (s). ^1H NMR (CD_2Cl_2): δ 19.11 (s, 1H, Ru=C*H*Ph), 7.37 (d, 6H, C*H* (*p*-$CF_3C_6H_4)_3P$, J_{HH} = 7 Hz), 7.32 (d, 2H, ortho C*H*, J_{HH} = 7 Hz), 7.29 (t, 1H, para C*H*, J_{HH} = 7 Hz), 7.04 (t, 8H, Mes C*H* and C*H* (*p*-$CF_3C_6H_4)_3P$, J_{HH} = 9 Hz), 6.77 (t, 2H, meta C*H*, J_{HH} = 8 Hz), 6.36 (s, 2H, Mes C*H*), 4.04 (m,

4H, CH_2CH_2), 2.61 (s, 6H, ortho CH_3), 2.44 (s, 3H, para CH_3), 2.22 (s, 6H, ortho CH_3), 1.93 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ 308.18-306.94 (multiple peaks, Ru=*C*HPh), 217.03 (d, Ru-*C*$(N)_2$, J_{CP} = 94 Hz), 151.60 (m), 139.82, 139.18, 138.77 (d), 137.44, 137.22, 135.46, 138.48 (t), 134.53, 134.23, 132.12 (q), 130.60, 130.51, 130.37, 130.29, 130.20 (d), 129.68 (d), 128.15, 127.99, 127.69 (d), 125.52, 125.13 (m), 123.26, 121.19, 52.60 (m), 51.81 (m), 21.24 (qu), 20.48 (q), 19.90, 18.69 (q). Anal. Calcd for $C_{49}H_{44}N_2F_9Cl_2PRu$: C, 56.87; H, 4.29; N, 2.71. Found: C, 56.99; H, 4.48; N, 2.60.

(IMesH$_2$)[(*p*-ClC$_6$H$_4$)$_3$P](Cl)$_2$Ru=CHPh (8). Complex **3** (60 mg, 0.083 mmol) and (*p*-$ClC_6H_4)_3P$ (60 mg, 0.164 mmol) were combined in benzene (2 mL) and stirred for 10 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 3 mL pentane and dried *in vacuo*. Complex **8** was obtained as a pink powder (54 mg, 70% yield). $^{31}P\{^1H\}$ NMR (C_6D_6): δ 37.10 (s). ^1H NMR (C_6D_6): δ 19.50 (s, 1H, Ru=C*H*Ph), 7.63 (d, 2H, ortho C*H*, J_{HH} = 8 Hz), 7.16-6.69 (multiple peaks, 17H, (*p*-$ClC_6H_4)_3P$, para C*H*, meta C*H*, and Mes C*H*), 6.30 (s, 2H, Mes C*H*), 3.31 (m, 4H, CH_2CH_2), 2.72 (s, 6H, ortho CH_3), 2.36 (s, 6H, ortho CH_3), 2.34 (s, 3H, para CH_3), 1.89 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (C_6D_6): δ 306.08 (m, Ru=*C*HPh), 218.53 (d, Ru-*C*$(N)_2$, J_{CP} = 93 Hz), 151.70 (d, J_{CP} = 3 Hz), 139.77, 138.94, 138.35, 137.70, 137.68 (d, J_{CP} = 2 Hz), 136.21, 135.67, 131.08, 130.46, 129.86, 129.75, 129.62, 129.32, 128.68, 128.03, 52.04 (d, J_{CP} = 4 Hz), 51.38 (d, J_{CP} = 2 Hz), 21.68, 21.31, 21.94, 19.06. Anal. Calcd for $C_{46}H_{44}N_2Cl_5PRu$: C, 59.14; H, 4.75; N, 3.00. Found: C, 58.77; H, 4.63; N, 3.22.

(IMesH$_2$)[(*p*-MeOC$_6$H$_4$)$_3$P](Cl)$_2$Ru=CHPh (9). Complex **3** (60 mg, 0.083 mmol) and (*p*-$MeOC_6H_4)_3P$ (45 mg, 0.13 mmol) were combined in benzene (2 mL) and stirred for 10 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 3 mL pentane and dried *in vacuo*. Complex **9** was obtained as a pink powder (45 mg, 59% yield). $^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ 35.52 (s). ^1H NMR (CD_2Cl_2): δ 19.16 (s, 1H, Ru=C*H*Ph), 7.41 (d, 2H, ortho C*H*, J_{HH} = 5 Hz), 7.36 (m, 2H, meta C*H*), 7.29 (t, 1H, para C*H*, J_{HH} = 5 Hz), 7.05 (s, 2H, Mes C*H*), 6.81 (m, 6H, C*H* (*p*-$MeOC_6H_4)_3P$), 6.61 (m, 6H, C*H* (*p*-$MeOC_6H_4)_3P$), 6.36 (s, 2H Mes C*H*), 4.00 (m, 4H, CH_2CH_2), 3.75 (s, 9H, OCH_3), 2.63 (s, 6H, ortho CH_3), 2.44 (s, 6H, ortho CH_3), 2.23 (s, 3H, para CH_3), 1.96 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ 303.85 (d, Ru=*C*HPh, J_{CP} = 9 Hz), 219.34 (d, Ru-*C*$(N)_2$, J_{CP} = 91 Hz), 161.14 (d, J_{CP} = 2 Hz),

151.10 (d, J_{CP} = 4 Hz), 139.61, 138.71, 138.34, 137.65, 137.40, 135.85 (d, J_{CP} = 13 Hz), 130.87, 130.08, 129.60, 129.24, 128.85, 127.81, 122.97, 122.62, 113.60 (d, J_{CP} = 10 Hz), 55.66, 52.56 (d, J_{CP} = 4 Hz), 51.78 (d, J_{CP} = 3 Hz), 21.65, 21.18, 20.48, 18.77. Anal. Calcd for $C_{49}H_{53}N_2Cl_2O_3PRu$: C, 63.91; H, 5.80; N, 3.04. Found: C, 64.49; H, 5.84; N, 3.03.

$(IMesH_2)(I)_2(C_5H_5N)Ru=CHPh$ (10). Complex **3** (60 mg, 0.083 mmol) and NaI (250 mg, 1.67 mmol) were combined in THF (4 mL) and stirred for 90 minutes. The volatiles were removed under vacuum, and the resulting residue was suspended in benzene and filtered through a plug of Celite. The solvent was removed under vacuum to afford complex **10** as a greenish solid (35 mg, 51% yield). ^{1}H NMR (C_6D_6): δ 19.24 (s, 1H, C*H*Ph), 8.37 (d, 2H, ortho C*H* (pyridine), J_{HH} = 5 Hz), 8.02 (d, 2H, ortho C*H*, J_{HH} = 7 Hz), 7.27 (t, 1H, para C*H*, J_{HH} = 7 Hz), 6.97-6.91 (multiple peaks, 4H, meta C*H*, Mes C*H*), 6.68 (s, 2H, Mes C*H*), 6.47 (t, 1H, para C*H* (pyridine), J_{HH} = 8 Hz), 6.13 (t, 2H, meta C*H* (pyridine), J_{HH} = 7 Hz), 3.43 (m, 4H, CH_2CH_2), 2.90 (s, 6H, ortho CH_3), 2.56 (s, 6H, ortho CH_3), 2.20 (s, 3H, para CH_3), 2.19 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (C_6D_6): δ 317.30 (m, Ru=*C*HPh), 219.91 (s, Ru-*C*$(N)_2$), 155.31, 151.75, 139.62, 139.22, 138.31, 138.15, 137.76, 136.22, 131.50, 131.43, 128.68, 123.39, 52.81, 51.19, 24.39, 21.52, 21.31, 20.92. Anal. Calcd for $C_{33}H_{37}N_3I_2Ru$: C, 47.72; H, 4.49; N, 5.06. Found: C, 47.11; H, 4.38; N, 5.73. Since the elemental analysis is outside the limits, complex **10** (10 mg, 0.012 mmol) was converted to the known compound $(IMesH_2)(I)_2(PCy_3)Ru=CHPh$[4] by addition of PCy_3 (10 mg, 0.036 mmol) in benzene (0.60 mL) in an NMR tube fitted with a screw cap. The NMR spectra of the product was identical to that of the known compound $(IMesH_2)(I)_2(PCy_3)Ru=CHPh$. This compound has acceptable elemental analysis: Anal. Calcd for $C_{46}H_{65}N_2I_2PRu$: C, 53.54; H, 6.35; N, 2.71. Found: C, 53.68; H, 6.32; N, 2.40.

References

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(2) Scholl, M.; Ding, S.; Lee, C. W.; Grubbs, R. H. *Org. Lett.* **1999**, *1*, 953.

(3) Sanford, M. S.; Ulman, M.; Grubbs, R. H. *J. Am. Chem. Soc.* **2001**, *123*, 749.

(4) Sanford, M. S.; Love, J. A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2001**, *123*, ASAP article.

Table 1. Crystal data and structure refinement for 3.

Empirical formula	C76 H84 Cl4 N8 Ru2
Formula weight	1453.46
Crystallization Solvent	Pentane/benzene
Crystal Habit	Rod
Crystal size	0.41 x 0.11 x 0.07 mm^3
Crystal color	Emerald green

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98 K	
θ range for 6912 reflections used in lattice determination	2.25 to 26.59°	
Unit cell dimensions	a = 12.3873(16) Å b = 15.529(2) Å c = 18.562(2) Å	α= 78.475(2)° β= 81.564(2)° γ = 76.745(2)°
Volume	3386.2(8) $Å^3$	
Z	4	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	2.758 Mg/m^3	
F(000)	1504	
Data collection program	Bruker SMART	
θ range for data collection	1.61 to 28.51°	
Completeness to θ = 28.51°	91.2 %	
Index ranges	$-16 \le h \le 16, -20 \le k \le 20, -24 \le l \le 24$	
Data collection scan type	ω scans at 7 ϕ settings	
Data reduction program	Bruker SAINT v.6.2	
Reflections collected	76469	
Independent reflections	15655 [R_{int}= 0.0867]	
Absorption coefficient	0.654 mm^{-1}	
Absorption correction	None	

Table 1 (cont.)

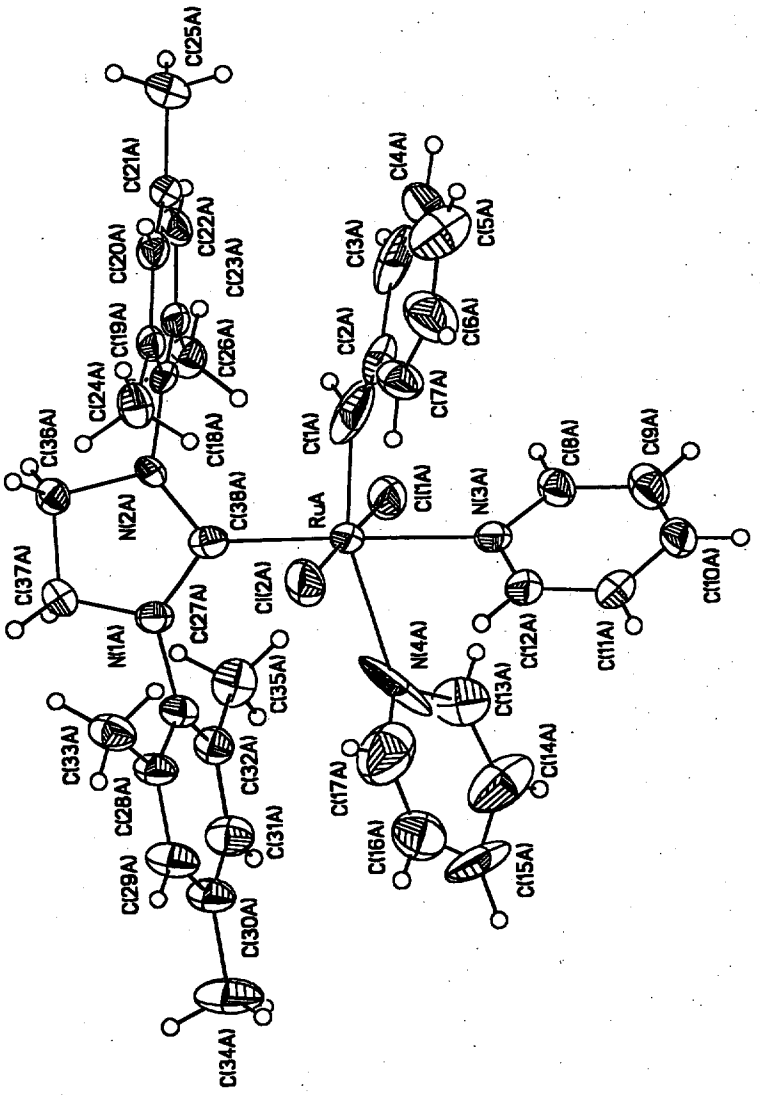
Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	15655 / 0 / 823
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.438
Final R indices [I>2σ(I), 9259 reflections]	R1 = 0.0609, *w*R2 = 0.0855
R indices (all data)	R1 = 0.1157, *w*R2 = 0.0904
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	2.095 and -1.363 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) 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 $F^2 > 2\sigma(F^2)$ 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.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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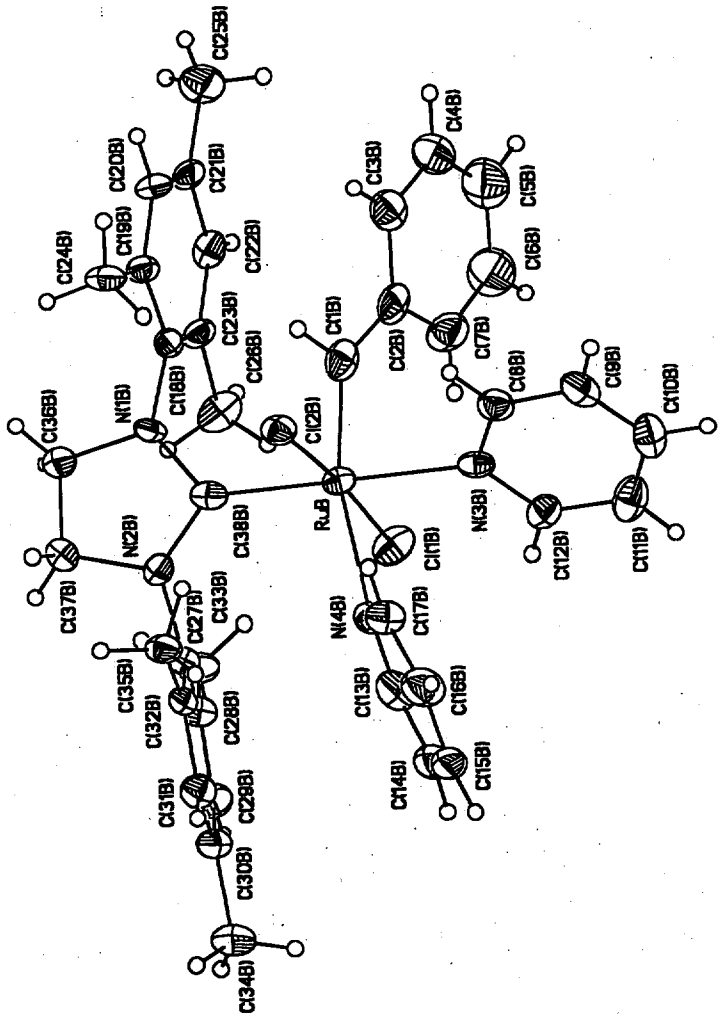
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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
RuA	3030(1)	5005(1)	2764(1)	34(1)
Cl(1A)	3436(1)	3896(1)	1947(1)	48(1)
Cl(2A)	2561(1)	6090(1)	3570(1)	54(1)
N(1A)	763(3)	5973(2)	2213(2)	30(1)
N(2A)	2116(3)	6377(2)	1448(2)	25(1)
N(3A)	4207(3)	4146(2)	3514(2)	33(1)
N(4A)	1938(4)	4069(5)	3540(3)	105(3)
C(1A)	4292(6)	5361(3)	2188(3)	74(2)
C(2A)	5111(5)	5654(3)	2321(3)	44(2)
C(3A)	6126(6)	5632(4)	1717(3)	67(2)
C(4A)	6981(4)	5957(4)	1899(3)	46(2)
C(5A)	6999(6)	6265(5)	2509(4)	97(3)
C(6A)	6174(5)	6235(4)	3007(4)	85(2)
C(7A)	5225(4)	5956(3)	2930(3)	42(1)
C(8A)	5081(4)	3545(3)	3285(3)	34(1)
C(9A)	5823(4)	2997(3)	3748(3)	43(1)
C(10A)	5683(4)	3063(3)	4479(3)	42(1)
C(11A)	4808(4)	3669(3)	4729(3)	44(1)
C(12A)	4088(4)	4197(3)	4230(3)	42(1)
C(13A)	2142(5)	3090(4)	3499(3)	50(2)
C(14A)	1626(5)	2452(4)	3967(3)	78(2)
C(15A)	817(5)	2783(5)	4579(3)	76(2)
C(16A)	753(5)	3703(4)	4564(4)	64(2)
C(17A)	1304(6)	4230(5)	4079(4)	95(3)
C(18A)	3142(3)	6603(3)	1081(2)	25(1)
C(19A)	3525(3)	7295(3)	1277(2)	28(1)
C(20A)	4445(3)	7578(3)	853(2)	29(1)
C(21A)	4968(3)	7208(3)	244(2)	29(1)
C(22A)	4558(3)	6540(3)	52(2)	30(1)
C(23A)	3643(3)	6228(3)	460(2)	25(1)
C(24A)	2960(3)	7723(3)	1932(2)	34(1)
C(25A)	5960(3)	7535(3)	-200(3)	46(1)
C(26A)	3209(4)	5497(3)	244(2)	34(1)
C(27A)	49(3)	5523(3)	2768(2)	30(1)
C(28A)	-546(4)	5971(3)	3332(3)	33(1)
C(29A)	-1300(4)	5561(3)	3821(3)	40(1)
C(30A)	-1489(4)	4725(3)	3766(3)	39(1)
C(31A)	-913(4)	4321(3)	3186(3)	40(1)
C(32A)	-158(4)	4705(3)	2687(2)	32(1)
C(33A)	-369(4)	6884(3)	3390(3)	38(1)
C(34A)	-2328(4)	4291(4)	4316(3)	63(2)
C(35A)	445(4)	4254(3)	2053(2)	44(1)
C(36A)	1113(3)	6940(3)	1115(2)	27(1)
C(37A)	186(3)	6563(3)	1609(2)	36(1)
C(38A)	1896(4)	5838(3)	2096(2)	28(1)
RuB	9078(1)	259(1)	2476(1)	21(1)
Cl(1B)	8372(1)	1556(1)	3055(1)	33(1)

Cl(2B)	9886(1)	-960(1)	1801(1)	26(1)
N(1B)	7236(3)	463(2)	1477(2)	21(1)
N(2B)	8382(3)	1328(2)	993(2)	23(1)
N(3B)	10163(3)	-326(2)	3366(2)	22(1)
N(4B)	10720(3)	834(2)	2059(2)	29(1)
C(1B)	8118(3)	-493(3)	2972(2)	32(1)
C(2B)	7517(4)	-641(3)	3682(3)	35(1)
C(3B)	7093(3)	-1454(3)	3911(2)	37(1)
C(4B)	6472(4)	-1603(4)	4573(3)	43(1)
C(5B)	6215(4)	-992(4)	5049(3)	61(2)
C(6B)	6605(4)	-214(4)	4846(3)	62(2)
C(7B)	7267(4)	-44(3)	4176(2)	39(1)
C(8B)	10562(3)	-1216(3)	3509(2)	28(1)
C(9B)	11207(3)	-1627(3)	4074(2)	32(1)
C(10B)	11468(3)	-1119(4)	4522(2)	36(1)
C(11B)	11080(3)	-202(3)	4374(2)	36(1)
C(12B)	10437(3)	170(3)	3797(2)	28(1)
C(13B)	10824(4)	1643(3)	2127(2)	37(1)
C(14B)	11829(4)	1888(3)	2038(2)	36(1)
C(15B)	12809(4)	1314(3)	1885(2)	34(1)
C(16B)	12723(4)	453(3)	1805(3)	43(1)
C(17B)	11681(3)	244(3)	1896(2)	29(1)
C(18B)	6487(3)	-13(3)	1987(2)	20(1)
C(19B)	6439(3)	-882(3)	1897(2)	22(1)
C(20B)	5652(3)	-1303(3)	2354(2)	25(1)
C(21B)	4921(3)	-895(3)	2887(2)	25(1)
C(22B)	4964(3)	-25(3)	2935(2)	26(1)
C(23B)	5717(3)	434(3)	2490(2)	23(1)
C(24B)	7221(3)	-1353(3)	1335(2)	29(1)
C(25B)	4089(3)	-1363(3)	3390(2)	40(1)
C(26B)	5707(3)	1380(3)	2550(3)	35(1)
C(27B)	9138(3)	1945(3)	858(2)	23(1)
C(28B)	8719(3)	2804(3)	1023(2)	25(1)
C(29B)	9389(3)	3423(3)	806(2)	29(1)
C(30B)	10454(3)	3232(3)	433(2)	25(1)
C(31B)	10818(3)	2371(3)	271(2)	26(1)
C(32B)	10189(3)	1720(3)	468(2)	21(1)
C(33B)	7567(3)	3048(3)	1420(2)	30(1)
C(34B)	11185(3)	3916(3)	232(2)	34(1)
C(35B)	10621(3)	813(3)	254(2)	27(1)
C(36B)	6792(3)	924(3)	777(2)	31(1)
C(37B)	7710(3)	1385(3)	386(2)	27(1)
C(38B)	8142(3)	747(3)	1615(2)	22(1)

Table 3. Selected bond lengths [Å] and angles [°] for 3.

RuA-C(1A)	1.887(7)	C(1A)-RuA-Cl(1A)	81.5(2)
RuA-C(38A)	2.053(4)	C(38A)-RuA-Cl(1A)	91.05(12)
RuA-N(3A)	2.192(4)	N(3A)-RuA-Cl(1A)	91.13(11)
RuA-N(4A)	2.348(7)	N(4A)-RuA-Cl(1A)	86.40(15)
RuA-Cl(2A)	2.3895(15)	Cl(2A)-RuA-Cl(1A)	177.90(5)
RuA-Cl(1A)	2.4389(15)	C(2A)-C(1A)-RuA	134.7(5)
C(1A)-C(2A)	1.277(7)	C(2A)-C(1A)-H(1A)	112.7
C(1A)-H(1A)	0.9300	RuA-C(1A)-H(1A)	112.7
RuB-C(1B)	1.873(4)	C(1B)-RuB-C(38B)	93.61(17)
RuB-C(38B)	2.033(4)	C(1B)-RuB-N(3B)	87.07(15)
RuB-N(3B)	2.203(3)	C(38B)-RuB-N(3B)	176.40(14)
RuB-N(4B)	2.372(4)	C(1B)-RuB-N(4B)	161.18(14)
RuB-Cl(1B)	2.3995(12)	C(38B)-RuB-N(4B)	102.85(14)
RuB-Cl(2B)	2.4227(12)	N(3B)-RuB-N(4B)	75.94(11)
C(1B)-C(2B)	1.420(6)	C(1B)-RuB-Cl(1B)	100.57(14)
C(1B)-H(1B)	0.9300	C(38B)-RuB-Cl(1B)	93.83(12)
		N(3B)-RuB-Cl(1B)	89.52(10)
C(1A)-RuA-C(38A)	95.1(2)	N(4B)-RuB-Cl(1B)	87.52(9)
C(1A)-RuA-N(3A)	86.0(2)	C(1B)-RuB-Cl(2B)	84.75(14)
C(38A)-RuA-N(3A)	177.68(16)	C(38B)-RuB-Cl(2B)	84.39(11)
C(1A)-RuA-N(4A)	159.0(2)	N(3B)-RuB-Cl(2B)	92.15(9)
C(38A)-RuA-N(4A)	102.19(17)	N(4B)-RuB-Cl(2B)	87.81(9)
N(3A)-RuA-N(4A)	77.16(14)	Cl(1B)-RuB-Cl(2B)	174.50(4)
C(1A)-RuA-Cl(2A)	100.3(2)	C(2B)-C(1B)-RuB	137.1(4)
C(38A)-RuA-Cl(2A)	87.78(12)	C(2B)-C(1B)-H(1B)	111.4
N(3A)-RuA-Cl(2A)	90.02(11)	RuB-C(1B)-H(1B)	111.4
N(4A)-RuA-Cl(2A)	92.14(15)		

Table 4. Bond lengths [Å] and angles [°] for 3.

RuA-C(1A)	1.887(7)	C(20A)-C(21A)	1.378(6)
RuA-C(38A)	2.053(4)	C(20A)-H(20A)	0.9300
RuA-N(3A)	2.192(4)	C(21A)-C(22A)	1.380(6)
RuA-N(4A)	2.348(7)	C(21A)-C(25A)	1.506(5)
RuA-Cl(2A)	2.3895(15)	C(22A)-C(23A)	1.395(5)
RuA-Cl(1A)	2.4389(15)	C(22A)-H(22A)	0.9300
N(1A)-C(38A)	1.362(5)	C(23A)-C(26A)	1.505(6)
N(1A)-C(27A)	1.436(5)	C(24A)-H(24A)	0.9600
N(1A)-C(37A)	1.460(5)	C(24A)-H(24B)	0.9600
N(2A)-C(38A)	1.352(5)	C(24A)-H(24C)	0.9600
N(2A)-C(18A)	1.434(5)	C(25A)-H(25A)	0.9600
N(2A)-C(36A)	1.484(5)	C(25A)-H(25B)	0.9600
N(3A)-C(12A)	1.332(5)	C(25A)-H(25C)	0.9600
N(3A)-C(8A)	1.336(5)	C(26A)-H(26A)	0.9600
N(4A)-C(17A)	1.208(8)	C(26A)-H(26B)	0.9600
N(4A)-C(13A)	1.498(8)	C(26A)-H(26C)	0.9600
C(1A)-C(2A)	1.277(7)	C(27A)-C(32A)	1.391(6)
C(1A)-H(1A)	0.9300	C(27A)-C(28A)	1.397(6)
C(2A)-C(7A)	1.343(7)	C(28A)-C(29A)	1.376(6)
C(2A)-C(3A)	1.555(7)	C(28A)-C(33A)	1.511(6)
C(3A)-C(4A)	1.382(7)	C(29A)-C(30A)	1.396(6)
C(3A)-H(3A)	0.9300	C(29A)-H(29A)	0.9300
C(4A)-C(5A)	1.319(8)	C(30A)-C(31A)	1.380(6)
C(4A)-H(4A)	0.9300	C(30A)-C(34A)	1.521(6)
C(5A)-C(6A)	1.275(8)	C(31A)-C(32A)	1.367(6)
C(5A)-H(5A)	0.9300	C(31A)-H(31A)	0.9300
C(6A)-C(7A)	1.377(7)	C(32A)-C(35A)	1.505(6)
C(6A)-H(6A)	0.9300	C(33A)-H(33A)	0.9600
C(7A)-H(7A)	0.9300	C(33A)-H(33B)	0.9600
C(8A)-C(9A)	1.375(6)	C(33A)-H(33C)	0.9600
C(8A)-H(8A)	0.9300	C(34A)-H(34A)	0.9600
C(9A)-C(10A)	1.364(6)	C(34A)-H(34B)	0.9600
C(9A)-H(9A)	0.9300	C(34A)-H(34C)	0.9600
C(10A)-C(11A)	1.355(6)	C(35A)-H(35A)	0.9600
C(10A)-H(10A)	0.9300	C(35A)-H(35B)	0.9600
C(11A)-C(12A)	1.389(6)	C(35A)-H(35C)	0.9600
C(11A)-H(11A)	0.9300	C(36A)-C(37A)	1.512(5)
C(12A)-H(12A)	0.9300	C(36A)-H(36A)	0.9700
C(13A)-C(14A)	1.389(7)	C(36A)-H(36B)	0.9700
C(13A)-H(13A)	0.9300	C(37A)-H(37A)	0.9700
C(14A)-C(15A)	1.492(8)	C(37A)-H(37B)	0.9700
C(14A)-H(14A)	0.9300	RuB-C(1B)	1.873(4)
C(15A)-C(16A)	1.409(8)	RuB-C(38B)	2.033(4)
C(15A)-H(15A)	0.9300	RuB-N(3B)	2.203(3)
C(16A)-C(17A)	1.315(8)	RuB-N(4B)	2.372(4)
C(16A)-H(16A)	0.9300	RuB-Cl(1B)	2.3995(12)
C(17A)-H(17A)	0.9300	RuB-Cl(2B)	2.4227(12)
C(18A)-C(23A)	1.394(5)	N(1B)-C(38B)	1.370(5)
C(18A)-C(19A)	1.397(6)	N(1B)-C(18B)	1.443(5)
C(19A)-C(20A)	1.393(5)	N(1B)-C(36B)	1.470(5)
C(19A)-C(24A)	1.507(5)	N(2B)-C(38B)	1.357(5)

N(2B)-C(27B)	1.450(5)	C(26B)-H(26D)	0.9600
N(2B)-C(37B)	1.474(5)	C(26B)-H(26E)	0.9600
N(3B)-C(12B)	1.340(5)	C(26B)-H(26F)	0.9600
N(3B)-C(8B)	1.344(5)	C(27B)-C(28B)	1.394(5)
N(4B)-C(13B)	1.324(5)	C(27B)-C(32B)	1.398(5)
N(4B)-C(17B)	1.362(5)	C(28B)-C(29B)	1.374(5)
C(1B)-C(2B)	1.420(6)	C(28B)-C(33B)	1.509(5)
C(1B)-H(1B)	0.9300	C(29B)-C(30B)	1.394(5)
C(2B)-C(7B)	1.387(6)	C(29B)-H(29B)	0.9300
C(2B)-C(3B)	1.441(6)	C(30B)-C(31B)	1.387(5)
C(3B)-C(4B)	1.360(6)	C(30B)-C(34B)	1.507(5)
C(3B)-H(3B)	0.9300	C(31B)-C(32B)	1.375(5)
C(4B)-C(5B)	1.378(7)	C(31B)-H(31B)	0.9300
C(4B)-H(4B)	0.9300	C(32B)-C(35B)	1.498(5)
C(5B)-C(6B)	1.366(7)	C(33B)-H(33D)	0.9600
C(5B)-H(5B)	0.9300	C(33B)-H(33E)	0.9600
C(6B)-C(7B)	1.399(6)	C(33B)-H(33F)	0.9600
C(6B)-H(6B)	0.9300	C(34B)-H(34D)	0.9600
C(7B)-H(7B)	0.9300	C(34B)-H(34E)	0.9600
C(8B)-C(9B)	1.375(5)	C(34B)-H(34F)	0.9600
C(8B)-H(8B)	0.9300	C(35B)-H(35D)	0.9600
C(9B)-C(10B)	1.369(6)	C(35B)-H(35E)	0.9600
C(9B)-H(9B)	0.9300	C(35B)-H(35F)	0.9600
C(10B)-C(11B)	1.380(6)	C(36B)-C(37B)	1.502(5)
C(10B)-H(10B)	0.9300	C(36B)-H(36C)	0.9700
C(11B)-C(12B)	1.380(5)	C(36B)-H(36D)	0.9700
C(11B)-H(11B)	0.9300	C(37B)-H(37C)	0.9700
C(12B)-H(12B)	0.9300	C(37B)-H(37D)	0.9700
C(13B)-C(14B)	1.362(6)		
C(13B)-H(13B)	0.9300	C(1A)-RuA-C(38A)	95.1(2)
C(14B)-C(15B)	1.361(6)	C(1A)-RuA-N(3A)	86.0(2)
C(14B)-H(14B)	0.9300	C(38A)-RuA-N(3A)	177.68(16)
C(15B)-C(16B)	1.403(6)	C(1A)-RuA-N(4A)	159.0(2)
C(15B)-H(15C)	0.9300	C(38A)-RuA-N(4A)	102.19(17)
C(16B)-C(17B)	1.381(5)	N(3A)-RuA-N(4A)	77.16(14)
C(16B)-H(16B)	0.9300	C(1A)-RuA-Cl(2A)	100.3(2)
C(17B)-H(17B)	0.9300	C(38A)-RuA-Cl(2A)	87.78(12)
C(18B)-C(23B)	1.398(5)	N(3A)-RuA-Cl(2A)	90.02(11)
C(18B)-C(19B)	1.408(5)	N(4A)-RuA-Cl(2A)	92.14(15)
C(19B)-C(20B)	1.388(5)	C(1A)-RuA-Cl(1A)	81.5(2)
C(19B)-C(24B)	1.498(5)	C(38A)-RuA-Cl(1A)	91.05(12)
C(20B)-C(21B)	1.387(5)	N(3A)-RuA-Cl(1A)	91.13(11)
C(20B)-H(20B)	0.9300	N(4A)-RuA-Cl(1A)	86.40(15)
C(21B)-C(22B)	1.386(6)	Cl(2A)-RuA-Cl(1A)	177.90(5)
C(21B)-C(25B)	1.500(5)	C(38A)-N(1A)-C(27A)	130.6(4)
C(22B)-C(23B)	1.380(5)	C(38A)-N(1A)-C(37A)	114.5(3)
C(22B)-H(22B)	0.9300	C(27A)-N(1A)-C(37A)	114.0(3)
C(23B)-C(26B)	1.492(5)	C(38A)-N(2A)-C(18A)	131.1(4)
C(24B)-H(24D)	0.9600	C(38A)-N(2A)-C(36A)	114.6(3)
C(24B)-H(24E)	0.9600	C(18A)-N(2A)-C(36A)	113.5(3)
C(24B)-H(24F)	0.9600	C(12A)-N(3A)-C(8A)	116.0(4)
C(25B)-H(25D)	0.9600	C(12A)-N(3A)-RuA	121.5(3)
C(25B)-H(25E)	0.9600	C(8A)-N(3A)-RuA	122.5(3)
C(25B)-H(25F)	0.9600	C(17A)-N(4A)-C(13A)	110.4(7)

C(17A)-N(4A)-RuA	127.8(7)	C(23A)-C(18A)-N(2A)	119.1(4)
C(13A)-N(4A)-RuA	120.8(3)	C(19A)-C(18A)-N(2A)	119.3(4)
C(2A)-C(1A)-RuA	134.7(5)	C(20A)-C(19A)-C(18A)	118.4(4)
C(2A)-C(1A)-H(1A)	112.7	C(20A)-C(19A)-C(24A)	120.7(4)
RuA-C(1A)-H(1A)	112.7	C(18A)-C(19A)-C(24A)	120.9(4)
C(1A)-C(2A)-C(7A)	128.2(6)	C(21A)-C(20A)-C(19A)	122.0(4)
C(1A)-C(2A)-C(3A)	116.3(6)	C(21A)-C(20A)-H(20A)	119.0
C(7A)-C(2A)-C(3A)	115.5(5)	C(19A)-C(20A)-H(20A)	119.0
C(4A)-C(3A)-C(2A)	113.2(5)	C(20A)-C(21A)-C(22A)	118.5(4)
C(4A)-C(3A)-H(3A)	123.4	C(20A)-C(21A)-C(25A)	120.4(4)
C(2A)-C(3A)-H(3A)	123.4	C(22A)-C(21A)-C(25A)	121.1(4)
C(5A)-C(4A)-C(3A)	126.7(6)	C(21A)-C(22A)-C(23A)	121.8(4)
C(5A)-C(4A)-H(4A)	116.7	C(21A)-C(22A)-H(22A)	119.1
C(3A)-C(4A)-H(4A)	116.7	C(23A)-C(22A)-H(22A)	119.1
C(6A)-C(5A)-C(4A)	118.4(8)	C(18A)-C(23A)-C(22A)	118.5(4)
C(6A)-C(5A)-H(5A)	120.8	C(18A)-C(23A)-C(26A)	120.4(4)
C(4A)-C(5A)-H(5A)	120.8	C(22A)-C(23A)-C(26A)	121.1(4)
C(5A)-C(6A)-C(7A)	124.1(8)	C(19A)-C(24A)-H(24A)	109.5
C(5A)-C(6A)-H(6A)	117.9	C(19A)-C(24A)-H(24B)	109.5
C(7A)-C(6A)-H(6A)	117.9	H(24A)-C(24A)-H(24B)	109.5
C(2A)-C(7A)-C(6A)	122.0(6)	C(19A)-C(24A)-H(24C)	109.5
C(2A)-C(7A)-H(7A)	119.0	H(24A)-C(24A)-H(24C)	109.5
C(6A)-C(7A)-H(7A)	119.0	H(24B)-C(24A)-H(24C)	109.5
N(3A)-C(8A)-C(9A)	123.3(5)	C(21A)-C(25A)-H(25A)	109.5
N(3A)-C(8A)-H(8A)	118.4	C(21A)-C(25A)-H(25B)	109.5
C(9A)-C(8A)-H(8A)	118.4	H(25A)-C(25A)-H(25B)	109.5
C(10A)-C(9A)-C(8A)	119.5(5)	C(21A)-C(25A)-H(25C)	109.5
C(10A)-C(9A)-H(9A)	120.3	H(25A)-C(25A)-H(25C)	109.5
C(8A)-C(9A)-H(9A)	120.3	H(25B)-C(25A)-H(25C)	109.5
C(11A)-C(10A)-C(9A)	118.8(5)	C(23A)-C(26A)-H(26A)	109.5
C(11A)-C(10A)-H(10A)	120.6	C(23A)-C(26A)-H(26B)	109.5
C(9A)-C(10A)-H(10A)	120.6	H(26A)-C(26A)-H(26B)	109.5
C(10A)-C(11A)-C(12A)	118.5(5)	C(23A)-C(26A)-H(26C)	109.5
C(10A)-C(11A)-H(11A)	120.8	H(26A)-C(26A)-H(26C)	109.5
C(12A)-C(11A)-H(11A)	120.8	H(26B)-C(26A)-H(26C)	109.5
N(3A)-C(12A)-C(11A)	123.9(5)	C(32A)-C(27A)-C(28A)	120.5(4)
N(3A)-C(12A)-H(12A)	118.0	C(32A)-C(27A)-N(1A)	119.9(4)
C(11A)-C(12A)-H(12A)	118.0	C(28A)-C(27A)-N(1A)	119.0(4)
C(14A)-C(13A)-N(4A)	126.4(5)	C(29A)-C(28A)-C(27A)	118.2(4)
C(14A)-C(13A)-H(13A)	116.8	C(29A)-C(28A)-C(33A)	121.5(4)
N(4A)-C(13A)-H(13A)	116.8	C(27A)-C(28A)-C(33A)	120.3(4)
C(13A)-C(14A)-C(15A)	115.8(6)	C(28A)-C(29A)-C(30A)	122.2(5)
C(13A)-C(14A)-H(14A)	122.1	C(28A)-C(29A)-H(29A)	118.9
C(15A)-C(14A)-H(14A)	122.1	C(30A)-C(29A)-H(29A)	118.9
C(16A)-C(15A)-C(14A)	111.1(5)	C(31A)-C(30A)-C(29A)	117.8(4)
C(16A)-C(15A)-H(15A)	124.4	C(31A)-C(30A)-C(34A)	121.3(5)
C(14A)-C(15A)-H(15A)	124.4	C(29A)-C(30A)-C(34A)	120.9(4)
C(17A)-C(16A)-C(15A)	126.3(7)	C(32A)-C(31A)-C(30A)	121.8(5)
C(17A)-C(16A)-H(16A)	116.9	C(32A)-C(31A)-H(31A)	119.1
C(15A)-C(16A)-H(16A)	116.9	C(30A)-C(31A)-H(31A)	119.1
N(4A)-C(17A)-C(16A)	129.9(9)	C(31A)-C(32A)-C(27A)	119.4(4)
N(4A)-C(17A)-H(17A)	115.1	C(31A)-C(32A)-C(35A)	120.6(4)
C(16A)-C(17A)-H(17A)	115.1	C(27A)-C(32A)-C(35A)	120.0(4)
C(23A)-C(18A)-C(19A)	120.8(4)	C(28A)-C(33A)-H(33A)	109.5

C(28A)-C(33A)-H(33B)	109.5
H(33A)-C(33A)-H(33B)	109.5
C(28A)-C(33A)-H(33C)	109.5
H(33A)-C(33A)-H(33C)	109.5
H(33B)-C(33A)-H(33C)	109.5
C(30A)-C(34A)-H(34A)	109.5
C(30A)-C(34A)-H(34B)	109.5
H(34A)-C(34A)-H(34B)	109.5
C(30A)-C(34A)-H(34C)	109.5
H(34A)-C(34A)-H(34C)	109.5
H(34B)-C(34A)-H(34C)	109.5
C(32A)-C(35A)-H(35A)	109.5
C(32A)-C(35A)-H(35B)	109.5
H(35A)-C(35A)-H(35B)	109.5
C(32A)-C(35A)-H(35C)	109.5
H(35A)-C(35A)-H(35C)	109.5
H(35B)-C(35A)-H(35C)	109.5
N(2A)-C(36A)-C(37A)	101.7(3)
N(2A)-C(36A)-H(36A)	111.4
C(37A)-C(36A)-H(36A)	111.4
N(2A)-C(36A)-H(36B)	111.4
C(37A)-C(36A)-H(36B)	111.4
H(36A)-C(36A)-H(36B)	109.3
N(1A)-C(37A)-C(36A)	103.0(3)
N(1A)-C(37A)-H(37A)	111.2
C(36A)-C(37A)-H(37A)	111.2
N(1A)-C(37A)-H(37B)	111.2
C(36A)-C(37A)-H(37B)	111.2
H(37A)-C(37A)-H(37B)	109.1
N(2A)-C(38A)-N(1A)	105.1(4)
N(2A)-C(38A)-RuA	127.3(3)
N(1A)-C(38A)-RuA	127.6(3)
C(1B)-RuB-C(38B)	93.61(17)
C(1B)-RuB-N(3B)	87.07(15)
C(38B)-RuB-N(3B)	176.40(14)
C(1B)-RuB-N(4B)	161.18(14)
C(38B)-RuB-N(4B)	102.85(14)
N(3B)-RuB-N(4B)	75.94(11)
C(1B)-RuB-Cl(1B)	100.57(14)
C(38B)-RuB-Cl(1B)	93.83(12)
N(3B)-RuB-Cl(1B)	89.52(10)
N(4B)-RuB-Cl(1B)	87.52(9)
C(1B)-RuB-Cl(2B)	84.75(14)
C(38B)-RuB-Cl(2B)	84.39(11)
N(3B)-RuB-Cl(2B)	92.15(9)
N(4B)-RuB-Cl(2B)	87.81(9)
Cl(1B)-RuB-Cl(2B)	174.50(4)
C(38B)-N(1B)-C(18B)	128.9(3)
C(38B)-N(1B)-C(36B)	113.9(3)
C(18B)-N(1B)-C(36B)	114.6(3)
C(38B)-N(2B)-C(27B)	129.6(3)
C(38B)-N(2B)-C(37B)	114.7(3)
C(27B)-N(2B)-C(37B)	115.5(3)
C(12B)-N(3B)-C(8B)	116.9(4)
C(12B)-N(3B)-RuB	122.7(3)
C(8B)-N(3B)-RuB	120.4(3)
C(13B)-N(4B)-C(17B)	116.4(4)
C(13B)-N(4B)-RuB	123.8(3)
C(17B)-N(4B)-RuB	118.0(3)
C(2B)-C(1B)-RuB	137.1(4)
C(2B)-C(1B)-H(1B)	111.4
RuB-C(1B)-H(1B)	111.4
C(7B)-C(2B)-C(1B)	124.9(5)
C(7B)-C(2B)-C(3B)	116.3(4)
C(1B)-C(2B)-C(3B)	118.8(5)
C(4B)-C(3B)-C(2B)	120.6(5)
C(4B)-C(3B)-H(3B)	119.7
C(2B)-C(3B)-H(3B)	119.7
C(3B)-C(4B)-C(5B)	122.1(5)
C(3B)-C(4B)-H(4B)	119.0
C(5B)-C(4B)-H(4B)	119.0
C(6B)-C(5B)-C(4B)	118.5(5)
C(6B)-C(5B)-H(5B)	120.7
C(4B)-C(5B)-H(5B)	120.7
C(5B)-C(6B)-C(7B)	121.1(6)
C(5B)-C(6B)-H(6B)	119.5
C(7B)-C(6B)-H(6B)	119.5
C(2B)-C(7B)-C(6B)	121.4(5)
C(2B)-C(7B)-H(7B)	119.3
C(6B)-C(7B)-H(7B)	119.3
N(3B)-C(8B)-C(9B)	123.3(4)
N(3B)-C(8B)-H(8B)	118.4
C(9B)-C(8B)-H(8B)	118.4
C(10B)-C(9B)-C(8B)	119.6(5)
C(10B)-C(9B)-H(9B)	120.2
C(8B)-C(9B)-H(9B)	120.2
C(9B)-C(10B)-C(11B)	117.8(4)
C(9B)-C(10B)-H(10B)	121.1
C(11B)-C(10B)-H(10B)	121.1
C(12B)-C(11B)-C(10B)	119.8(4)
C(12B)-C(11B)-H(11B)	120.1
C(10B)-C(11B)-H(11B)	120.1
N(3B)-C(12B)-C(11B)	122.6(4)
N(3B)-C(12B)-H(12B)	118.7
C(11B)-C(12B)-H(12B)	118.7
N(4B)-C(13B)-C(14B)	122.8(5)
N(4B)-C(13B)-H(13B)	118.6
C(14B)-C(13B)-H(13B)	118.6
C(15B)-C(14B)-C(13B)	122.5(5)
C(15B)-C(14B)-H(14B)	118.7
C(13B)-C(14B)-H(14B)	118.7
C(14B)-C(15B)-C(16B)	115.9(4)
C(14B)-C(15B)-H(15C)	122.0
C(16B)-C(15B)-H(15C)	122.0
C(17B)-C(16B)-C(15B)	119.0(5)
C(17B)-C(16B)-H(16B)	120.5
C(15B)-C(16B)-H(16B)	120.5
N(4B)-C(17B)-C(16B)	123.3(4)

N(4B)-C(17B)-H(17B)	118.4	C(28B)-C(29B)-H(29B)	118.4
C(16B)-C(17B)-H(17B)	118.4	C(30B)-C(29B)-H(29B)	118.4
C(23B)-C(18B)-C(19B)	120.9(4)	C(31B)-C(30B)-C(29B)	116.5(4)
C(23B)-C(18B)-N(1B)	119.9(4)	C(31B)-C(30B)-C(34B)	121.7(4)
C(19B)-C(18B)-N(1B)	118.6(4)	C(29B)-C(30B)-C(34B)	121.8(4)
C(20B)-C(19B)-C(18B)	118.0(4)	C(32B)-C(31B)-C(30B)	123.2(4)
C(20B)-C(19B)-C(24B)	120.4(4)	C(32B)-C(31B)-H(31B)	118.4
C(18B)-C(19B)-C(24B)	121.6(4)	C(30B)-C(31B)-H(31B)	118.4
C(21B)-C(20B)-C(19B)	122.3(4)	C(31B)-C(32B)-C(27B)	117.7(4)
C(21B)-C(20B)-H(20B)	118.9	C(31B)-C(32B)-C(35B)	120.3(4)
C(19B)-C(20B)-H(20B)	118.9	C(27B)-C(32B)-C(35B)	122.0(4)
C(22B)-C(21B)-C(20B)	117.8(4)	C(28B)-C(33B)-H(33D)	109.5
C(22B)-C(21B)-C(25B)	120.3(4)	C(28B)-C(33B)-H(33E)	109.5
C(20B)-C(21B)-C(25B)	121.9(4)	H(33D)-C(33B)-H(33E)	109.5
C(23B)-C(22B)-C(21B)	122.7(4)	C(28B)-C(33B)-H(33F)	109.5
C(23B)-C(22B)-H(22B)	118.7	H(33D)-C(33B)-H(33F)	109.5
C(21B)-C(22B)-H(22B)	118.7	H(33E)-C(33B)-H(33F)	109.5
C(22B)-C(23B)-C(18B)	118.2(4)	C(30B)-C(34B)-H(34D)	109.5
C(22B)-C(23B)-C(26B)	120.5(4)	C(30B)-C(34B)-H(34E)	109.5
C(18B)-C(23B)-C(26B)	121.3(4)	H(34D)-C(34B)-H(34E)	109.5
C(19B)-C(24B)-H(24D)	109.5	C(30B)-C(34B)-H(34F)	109.5
C(19B)-C(24B)-H(24E)	109.5	H(34D)-C(34B)-H(34F)	109.5
H(24D)-C(24B)-H(24E)	109.5	H(34E)-C(34B)-H(34F)	109.5
C(19B)-C(24B)-H(24F)	109.5	C(32B)-C(35B)-H(35D)	109.5
H(24D)-C(24B)-H(24F)	109.5	C(32B)-C(35B)-H(35E)	109.5
H(24E)-C(24B)-H(24F)	109.5	H(35D)-C(35B)-H(35E)	109.5
C(21B)-C(25B)-H(25D)	109.5	C(32B)-C(35B)-H(35F)	109.5
C(21B)-C(25B)-H(25E)	109.5	H(35D)-C(35B)-H(35F)	109.5
H(25D)-C(25B)-H(25E)	109.5	H(35E)-C(35B)-H(35F)	109.5
C(21B)-C(25B)-H(25F)	109.5	N(1B)-C(36B)-C(37B)	102.5(3)
H(25D)-C(25B)-H(25F)	109.5	N(1B)-C(36B)-H(36C)	111.3
H(25E)-C(25B)-H(25F)	109.5	C(37B)-C(36B)-H(36C)	111.3
C(23B)-C(26B)-H(26D)	109.5	N(1B)-C(36B)-H(36D)	111.3
C(23B)-C(26B)-H(26E)	109.5	C(37B)-C(36B)-H(36D)	111.3
H(26D)-C(26B)-H(26E)	109.5	H(36C)-C(36B)-H(36D)	109.2
C(23B)-C(26B)-H(26F)	109.5	N(2B)-C(37B)-C(36B)	101.8(3)
H(26D)-C(26B)-H(26F)	109.5	N(2B)-C(37B)-H(37C)	111.4
H(26E)-C(26B)-H(26F)	109.5	C(36B)-C(37B)-H(37C)	111.4
C(28B)-C(27B)-C(32B)	121.7(4)	N(2B)-C(37B)-H(37D)	111.4
C(28B)-C(27B)-N(2B)	117.7(4)	C(36B)-C(37B)-H(37D)	111.4
C(32B)-C(27B)-N(2B)	119.8(4)	H(37C)-C(37B)-H(37D)	109.3
C(29B)-C(28B)-C(27B)	117.6(4)	N(2B)-C(38B)-N(1B)	104.5(3)
C(29B)-C(28B)-C(33B)	121.2(4)	N(2B)-C(38B)-RuB	127.0(3)
C(27B)-C(28B)-C(33B)	121.2(4)	N(1B)-C(38B)-RuB	127.8(3)
C(28B)-C(29B)-C(30B)	123.2(4)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) 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}
RuA	249(2)	311(3)	355(3)	53(2)	62(2)	7(2)
Cl(1A)	450(8)	446(9)	393(8)	8(7)	54(6)	103(7)
Cl(2A)	470(8)	608(10)	321(7)	-51(7)	76(6)	214(7)
N(1A)	270(20)	260(20)	330(20)	-22(18)	51(18)	-58(18)
N(2A)	180(19)	220(20)	290(20)	-45(18)	39(16)	34(16)
N(3A)	290(20)	260(20)	360(20)	10(20)	89(19)	-25(19)
N(4A)	150(30)	2440(90)	500(40)	-700(50)	-20(20)	230(40)
C(1A)	1230(60)	230(40)	530(40)	110(30)	-20(40)	110(40)
C(2A)	600(40)	260(30)	430(40)	100(30)	-230(30)	-80(30)
C(3A)	1140(60)	470(40)	320(30)	90(30)	-320(40)	10(40)
C(4A)	340(30)	620(40)	390(30)	-150(30)	-80(30)	40(30)
C(5A)	990(60)	910(60)	810(60)	230(50)	90(50)	-210(50)
C(6A)	390(40)	570(50)	1480(70)	80(50)	-10(40)	-140(30)
C(7A)	300(30)	350(30)	640(40)	-110(30)	30(30)	-110(20)
C(8A)	280(30)	220(30)	490(30)	-70(20)	0(20)	-20(20)
C(9A)	320(30)	270(30)	710(40)	-70(30)	-90(30)	-50(20)
C(10A)	270(30)	330(30)	620(40)	70(30)	-80(30)	-80(20)
C(11A)	430(30)	390(30)	380(30)	90(30)	10(30)	-60(30)
C(12A)	360(30)	390(30)	380(30)	60(30)	80(30)	30(20)
C(13A)	640(40)	450(40)	490(40)	-310(30)	80(30)	-150(30)
C(14A)	1070(50)	900(50)	570(40)	160(40)	-340(40)	-690(50)
C(15A)	810(50)	1260(70)	310(30)	350(40)	-190(30)	-740(50)
C(16A)	470(40)	690(50)	810(50)	-50(40)	-130(30)	-220(40)
C(17A)	870(60)	1020(70)	990(60)	320(50)	-420(50)	-460(50)
C(18A)	280(30)	160(30)	260(30)	50(20)	0(20)	0(20)
C(19A)	270(30)	230(30)	260(30)	-10(20)	-10(20)	60(20)
C(20A)	290(30)	200(30)	360(30)	0(20)	-80(20)	-50(20)
C(21A)	230(30)	280(30)	300(30)	50(20)	-10(20)	-30(20)
C(22A)	250(30)	290(30)	290(30)	-70(20)	10(20)	90(20)
C(23A)	250(20)	180(30)	250(30)	-10(20)	0(20)	20(20)
C(24A)	350(30)	290(30)	380(30)	-110(20)	-80(20)	30(20)
C(25A)	260(30)	530(40)	530(30)	10(30)	50(20)	-90(30)
C(26A)	390(30)	240(30)	360(30)	-110(20)	-20(20)	10(20)
C(27A)	230(30)	320(30)	330(30)	-40(20)	10(20)	-90(20)
C(28A)	270(30)	330(30)	410(30)	-80(20)	50(20)	-130(20)
C(29A)	350(30)	440(30)	480(30)	-200(30)	100(20)	-190(30)
C(30A)	320(30)	410(30)	460(30)	-100(30)	60(20)	-180(30)
C(31A)	420(30)	380(30)	460(30)	-110(30)	-10(30)	-180(30)
C(32A)	320(30)	310(30)	310(30)	-100(20)	0(20)	-30(20)
C(33A)	320(30)	340(30)	490(30)	-150(30)	90(20)	-90(20)
C(34A)	590(40)	640(40)	740(40)	-240(30)	250(30)	-410(30)
C(35A)	530(30)	410(30)	390(30)	-110(30)	-90(30)	-70(30)
C(36A)	280(30)	210(30)	290(30)	-80(20)	0(20)	0(20)
C(37A)	240(30)	370(30)	410(30)	-20(20)	-30(20)	10(20)
C(38A)	310(30)	190(30)	310(30)	-100(20)	80(20)	-40(20)
RuB	180(2)	199(2)	249(2)	-44(2)	1(2)	-61(2)
Cl(1B)	266(6)	286(7)	464(8)	-167(6)	-26(5)	-26(5)

Cl(2B)	313(6)	197(6)	271(6)	-60(5)	-10(5)	-57(5)
N(1B)	216(19)	170(20)	220(20)	29(16)	-5(15)	-67(16)
N(2B)	220(20)	240(20)	240(20)	-49(17)	-51(16)	-69(17)
N(3B)	183(19)	200(20)	250(20)	-50(18)	68(16)	-73(17)
N(4B)	470(30)	150(20)	260(20)	-39(18)	-57(19)	-82(19)
C(1B)	250(30)	340(30)	380(30)	-60(20)	-140(20)	20(20)
C(2B)	200(30)	500(40)	380(30)	-40(30)	-130(20)	-100(20)
C(3B)	260(30)	460(40)	350(30)	-10(30)	-60(20)	-70(20)
C(4B)	450(30)	520(40)	330(30)	-20(30)	30(30)	-200(30)
C(5B)	460(40)	920(50)	450(40)	-40(40)	40(30)	-260(40)
C(6B)	570(40)	950(50)	400(30)	-150(30)	120(30)	-360(40)
C(7B)	320(30)	520(40)	370(30)	-140(30)	60(20)	-200(30)
C(8B)	260(30)	290(30)	270(30)	-20(20)	20(20)	-100(20)
C(9B)	260(30)	310(30)	330(30)	60(20)	-10(20)	-40(20)
C(10B)	210(30)	590(40)	250(30)	-40(30)	-20(20)	-40(30)
C(11B)	290(30)	500(40)	330(30)	-180(30)	-30(20)	-60(30)
C(12B)	270(30)	280(30)	290(30)	-90(20)	-20(20)	-80(20)
C(13B)	380(30)	350(30)	330(30)	10(20)	-30(20)	-50(30)
C(14B)	300(30)	410(30)	350(30)	30(20)	-40(20)	-140(30)
C(15B)	290(30)	380(30)	370(30)	60(30)	-100(20)	-150(30)
C(16B)	320(30)	450(40)	480(30)	80(30)	-70(20)	-120(30)
C(17B)	240(30)	250(30)	350(30)	-40(20)	10(20)	-40(20)
C(18B)	140(20)	260(30)	210(20)	0(20)	-29(18)	-50(20)
C(19B)	200(20)	230(30)	250(20)	-20(20)	-10(19)	-80(20)
C(20B)	250(20)	220(30)	320(30)	-50(20)	0(20)	-120(20)
C(21B)	170(20)	350(30)	260(30)	-50(20)	-5(19)	-140(20)
C(22B)	210(20)	350(30)	240(30)	-130(20)	13(19)	-50(20)
C(23B)	170(20)	250(30)	300(30)	-30(20)	-50(20)	-90(20)
C(24B)	340(30)	250(30)	290(30)	-70(20)	90(20)	-160(20)
C(25B)	320(30)	520(40)	380(30)	-70(30)	100(20)	-180(30)
C(26B)	240(30)	330(30)	520(30)	-190(30)	-30(20)	-20(20)
C(27B)	260(30)	240(30)	200(20)	0(20)	-39(19)	-100(20)
C(28B)	250(20)	220(30)	270(30)	-20(20)	0(20)	-70(20)
C(29B)	290(30)	230(30)	340(30)	-90(20)	-20(20)	-50(20)
C(30B)	250(30)	220(30)	290(30)	-20(20)	-20(20)	-70(20)
C(31B)	210(20)	280(30)	290(30)	-40(20)	0(20)	-50(20)
C(32B)	270(20)	180(30)	180(20)	4(19)	-48(19)	-70(20)
C(33B)	300(30)	200(30)	390(30)	-60(20)	20(20)	-60(20)
C(34B)	320(30)	300(30)	390(30)	-40(20)	60(20)	-120(20)
C(35B)	370(30)	250(30)	220(20)	-70(20)	50(20)	-140(20)
C(36B)	310(30)	320(30)	320(30)	40(20)	-90(20)	-150(20)
C(37B)	310(30)	270(30)	240(30)	10(20)	-50(20)	-90(20)
C(38B)	210(20)	180(30)	250(20)	-70(20)	67(19)	-40(20)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 3.

	x	y	z	U_{iso}
H(1A)	4324	5311	1694	89
H(3A)	6154	5421	1279	81
H(4A)	7609	5959	1556	55
H(5A)	7598	6499	2574	117
H(6A)	6217	6412	3450	102
H(7A)	4646	5978	3310	51
H(8A)	5193	3495	2787	41
H(9A)	6416	2584	3564	52
H(10A)	6179	2699	4799	50
H(11A)	4693	3731	5225	52
H(12A)	3488	4609	4406	51
H(13A)	2666	2890	3123	60
H(14A)	1775	1855	3902	93
H(15A)	408	2427	4926	91
H(16A)	275	3964	4933	77
H(17A)	1188	4817	4163	114
H(20A)	4715	8030	985	34
H(22A)	4901	6291	-360	36
H(24A)	2182	7946	1876	51
H(24B)	3297	8212	1962	51
H(24C)	3042	7286	2377	51
H(25A)	6586	7349	85	70
H(25B)	5785	8178	-323	70
H(25C)	6140	7284	-646	70
H(26A)	3200	5011	654	51
H(26B)	3685	5282	-168	51
H(26C)	2466	5731	107	51
H(29A)	-1697	5851	4201	48
H(31A)	-1041	3771	3133	48
H(33A)	-861	7103	3794	58
H(33B)	-525	7293	2939	58
H(33C)	390	6836	3475	58
H(34A)	-2183	4289	4810	94
H(34B)	-2263	3685	4245	94
H(34C)	-3069	4625	4239	94
H(35A)	206	3702	2077	66
H(35B)	1234	4130	2085	66
H(35C)	278	4643	1594	66
H(36A)	1123	6868	606	32
H(36B)	1047	7570	1133	32
H(37A)	-382	7037	1789	44
H(37B)	-157	6229	1350	44
H(1B)	8006	-871	2672	39
H(3B)	7245	-1881	3602	44
H(4B)	6212	-2135	4710	52
H(5B)	5786	-1106	5499	73
H(6B)	6427	210	5158	74
H(7B)	7546	480	4060	46

H(8B)	10394	-1572	3211	33
H(9B)	11465	-2247	4152	38
H(10B)	11892	-1383	4912	43
H(11B)	11251	165	4662	43
H(12B)	10185	790	3704	33
H(13B)	10184	2061	2241	44
H(14B)	11847	2471	2083	43
H(15C)	13494	1482	1836	41
H(16B)	13359	29	1693	52
H(17B)	11634	-329	1843	35
H(20B)	5614	-1878	2302	30
H(22B)	4465	262	3281	32
H(24D)	7167	-1973	1421	43
H(24E)	7971	-1313	1375	43
H(24F)	7026	-1074	848	43
H(25D)	3348	-1035	3307	60
H(25E)	4207	-1393	3895	60
H(25F)	4181	-1960	3289	60
H(26D)	6397	1408	2712	53
H(26E)	5098	1584	2900	53
H(26F)	5619	1756	2076	53
H(29B)	9118	3999	913	35
H(31B)	11522	2226	17	32
H(33D)	7418	3666	1478	45
H(33E)	7525	2673	1898	45
H(33F)	7025	2959	1136	45
H(34D)	11697	3811	597	51
H(34E)	10729	4508	215	51
H(34F)	11594	3863	-244	51
H(35D)	10428	825	-231	41
H(35E)	10294	374	603	41
H(35F)	11417	660	252	41
H(36C)	6104	1354	862	37
H(36D)	6661	499	497	37
H(37C)	8140	1074	-1	33
H(37D)	7418	2004	174	33