Salicylaldimine Ruthenium Alkylidene Complexes: Metathesis Catalysts Tuned for Protic Solvents

Joseph B. Binder, Ilia A. Guzei, and Ronald T. Raines*

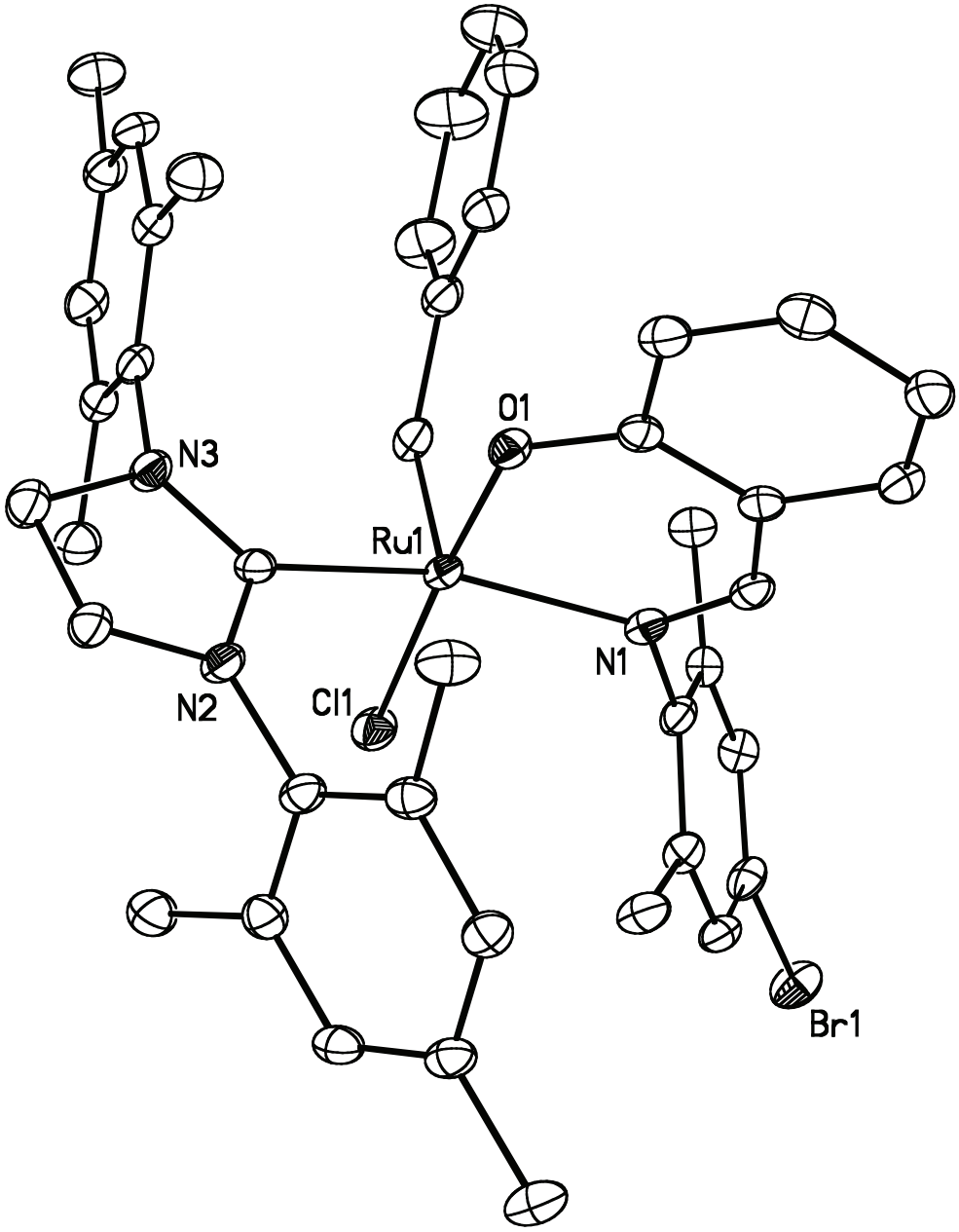

Figure 1S. Solid-state molecular structure of complex **7a**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are shown at 50% probability.

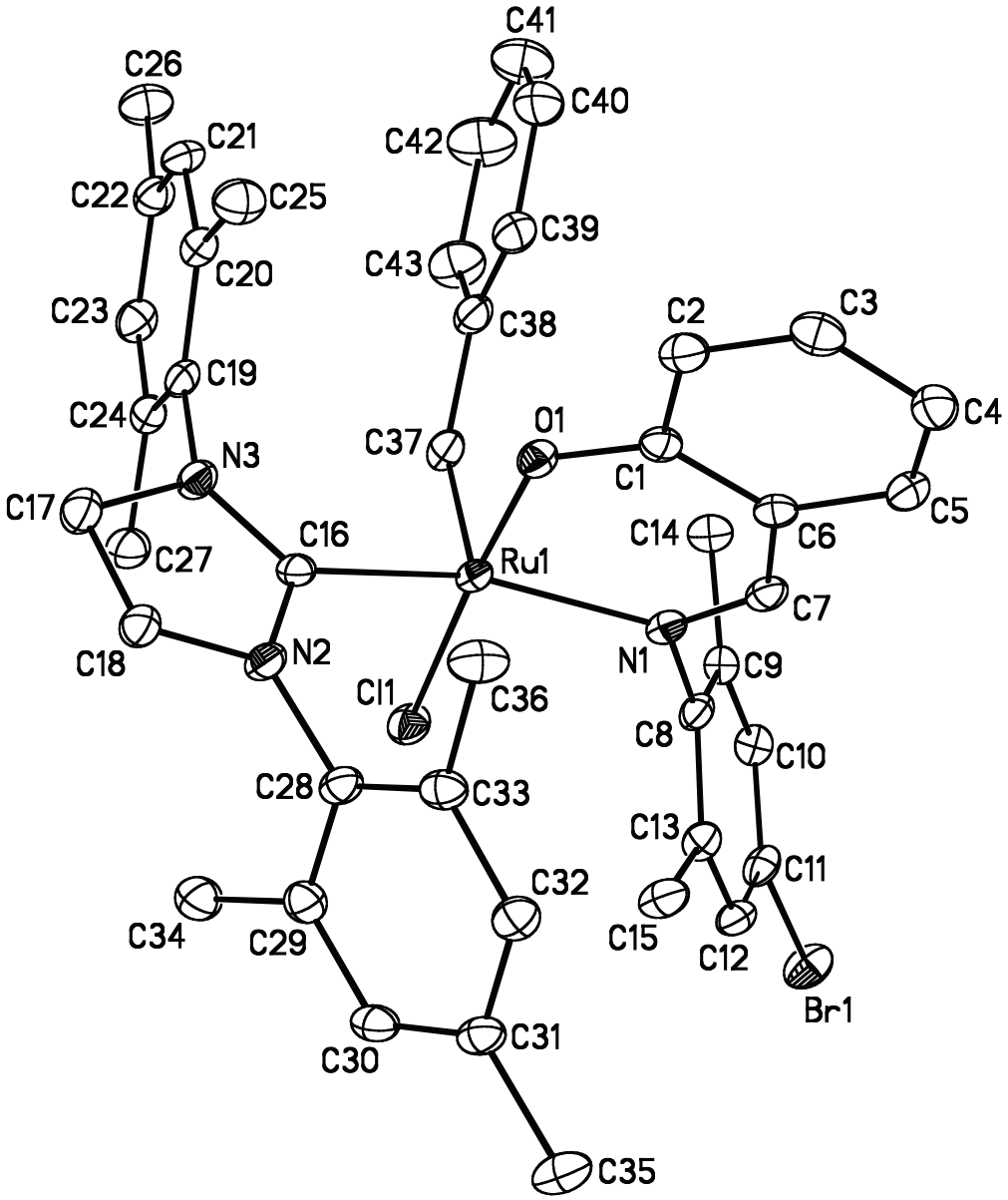

Figure 2S. Solid-state molecular structure of complex **7a**. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are shown at 50% probability.

Table S1. Crystal data and structure refinement of complex **7a**.

Identification code	raines05	
Empirical formula	$C_{43}H_{45}BrClN_3ORu$	
Formula weight	836.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.2903(8) Å	α = 107.0270(10)°
	b = 11.3962(8) Å	β = 90.5140(10)°
	c = 16.3627(12) Å	γ = 110.8190(10)°
Volume	1866.5(2) Å^3	
Z	2	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	1.600 mm^{-1}	
F(000)	856	
Crystal size	0.36 × 0.31 × 0.30 mm^3	
Theta range for data collection	1.31 to 26.39°	
Index ranges	$-14 \le h \le 14$, $-14 \le k \le 14$, $-20 \le l \le 20$	
Reflections collected	27052	
Independent reflections	7597 [R(int) = 0.0252]	
Completeness to theta = 26.39°	99.4%	
Absorption correction	Multi-scan with SADABS	
Max. and min. transmission	0.6454 and 0.5966	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7597 / 0 / 459	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	$R1$ = 0.0262, $wR2$ = 0.0662	
R indices (all data)	$R1$ = 0.0335, $wR2$ = 0.0739	
Largest diff. peak and hole	0.925 and –0.396 e.Å^{-3}	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of complex **7a**. *U*(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	*y*	*z*	*U*(eq)
Ru(1)	6706(1)	9153(1)	2513(1)	14(1)
Br(1)	1145(1)	2716(1)	1665(1)	26(1)
Cl(1)	6017(1)	7643(1)	3327(1)	22(1)
O(1)	7410(1)	10286(1)	1727(1)	16(1)
N(1)	5202(2)	7849(2)	1528(1)	16(1)
N(2)	9405(2)	9574(2)	2856(1)	17(1)
N(3)	9121(2)	11259(2)	3741(1)	17(1)
C(1)	7012(2)	10059(2)	926(1)	16(1)
C(2)	7702(2)	10975(2)	510(2)	19(1)
C(3)	7386(2)	10780(2)	-341(2)	21(1)
C(4)	6342(2)	9662(2)	-841(2)	21(1)
C(5)	5635(2)	8787(2)	-449(1)	19(1)
C(6)	5933(2)	8943(2)	429(1)	16(1)
C(7)	5125(2)	7959(2)	762(1)	17(1)
C(8)	4242(2)	6665(2)	1611(1)	16(1)
C(9)	3092(2)	6684(2)	1912(1)	17(1)
C(10)	2169(2)	5496(2)	1936(1)	18(1)
C(11)	2417(2)	4348(2)	1668(1)	19(1)
C(12)	3561(2)	4331(2)	1391(1)	19(1)
C(13)	4499(2)	5503(2)	1362(1)	17(1)
C(14)	2844(2)	7948(2)	2219(2)	21(1)
C(15)	5779(2)	5526(2)	1100(2)	22(1)
C(16)	8514(2)	10075(2)	3139(1)	15(1)
C(17)	10498(2)	11565(2)	3937(2)	22(1)
C(18)	10723(2)	10503(2)	3207(2)	19(1)
C(19)	8542(2)	12092(2)	4284(1)	16(1)
C(20)	8664(2)	13280(2)	4147(1)	18(1)
C(21)	8110(2)	14077(2)	4685(2)	20(1)
C(22)	7442(2)	13715(2)	5338(2)	20(1)
C(23)	7365(2)	12542(2)	5468(1)	21(1)
C(24)	7919(2)	11715(2)	4954(1)	19(1)
C(25)	9340(2)	13679(2)	3426(2)	24(1)
C(26)	6792(2)	14561(2)	5878(2)	27(1)
C(27)	7821(2)	10450(2)	5115(2)	24(1)
C(28)	9173(2)	8281(2)	2255(1)	17(1)
C(29)	8989(2)	7224(2)	2578(2)	19(1)
C(30)	8820(2)	5994(2)	1994(2)	19(1)
C(31)	8828(2)	5790(2)	1115(2)	19(1)
C(32)	9046(2)	6860(2)	819(2)	19(1)
C(33)	9246(2)	8127(2)	1378(2)	18(1)
C(34)	8979(2)	7388(2)	3527(2)	25(1)
C(35)	8582(2)	4424(2)	504(2)	26(1)
C(36)	9574(2)	9273(2)	1029(2)	23(1)
C(37)	5970(2)	10202(2)	3222(1)	19(1)
C(38)	5700(2)	11372(2)	3206(2)	20(1)
C(39)	6186(2)	12132(2)	2666(2)	23(1)
C(40)	5873(3)	13216(3)	2700(2)	29(1)
C(41)	5058(3)	13554(3)	3269(2)	38(1)
C(42)	4575(3)	12827(3)	3814(2)	40(1)
C(43)	4898(2)	11745(3)	3790(2)	30(1)

Table S3. Bond lengths [Å] and angles [°] of complex **7a**.

Ru(1)-C(37)	1.838(2)	C(20)-C(25)	1.505(3)
Ru(1)-C(16)	2.032(2)	C(21)-C(22)	1.389(3)
Ru(1)-O(1)	2.0530(15)	C(21)-H(21)	0.9500
Ru(1)-N(1)	2.1080(18)	C(22)-C(23)	1.388(3)
Ru(1)-Cl(1)	2.3976(6)	C(22)-C(26)	1.506(3)
Br(1)-C(11)	1.902(2)	C(23)-C(24)	1.397(3)
O(1)-C(1)	1.301(3)	C(23)-H(23)	0.9500
N(1)-C(7)	1.301(3)	C(24)-C(27)	1.506(3)
N(1)-C(8)	1.444(3)	C(25)-H(25A)	0.9800
N(2)-C(16)	1.347(3)	C(25)-H(25B)	0.9800
N(2)-C(28)	1.442(3)	C(25)-H(25C)	0.9800
N(2)-C(18)	1.475(3)	C(26)-H(26A)	0.9800
N(3)-C(16)	1.346(3)	C(26)-H(26B)	0.9800
N(3)-C(19)	1.441(3)	C(26)-H(26C)	0.9800
N(3)-C(17)	1.477(3)	C(27)-H(27A)	0.9800
C(1)-C(2)	1.417(3)	C(27)-H(27B)	0.9800
C(1)-C(6)	1.428(3)	C(27)-H(27C)	0.9800
C(2)-C(3)	1.367(3)	C(28)-C(33)	1.400(3)
C(2)-H(2)	0.9500	C(28)-C(29)	1.404(3)
C(3)-C(4)	1.410(3)	C(29)-C(30)	1.392(3)
C(3)-H(3)	0.9500	C(29)-C(34)	1.510(3)
C(4)-C(5)	1.364(3)	C(30)-C(31)	1.388(3)
C(4)-H(4)	0.9500	C(30)-H(30)	0.9500
C(5)-C(6)	1.417(3)	C(31)-C(32)	1.384(3)
C(5)-H(5)	0.9500	C(31)-C(35)	1.509(3)
C(6)-C(7)	1.423(3)	C(32)-C(33)	1.402(3)
C(7)-H(7)	0.9500	C(32)-H(32)	0.9500
C(8)-C(9)	1.398(3)	C(33)-C(36)	1.505(3)
C(8)-C(13)	1.401(3)	C(34)-H(34A)	0.9800
C(9)-C(10)	1.396(3)	C(34)-H(34B)	0.9800
C(9)-C(14)	1.507(3)	C(34)-H(34C)	0.9800
C(10)-C(11)	1.381(3)	C(35)-H(35A)	0.9800
C(10)-H(10)	0.9500	C(35)-H(35B)	0.9800
C(11)-C(12)	1.377(3)	C(35)-H(35C)	0.9800
C(12)-C(13)	1.393(3)	C(36)-H(36A)	0.9800
C(12)-H(12)	0.9500	C(36)-H(36B)	0.9800
C(13)-C(15)	1.505(3)	C(36)-H(36C)	0.9800
C(14)-H(14A)	0.9800	C(37)-C(38)	1.476(3)
C(14)-H(14B)	0.9800	C(37)-H(37)	0.9500
C(14)-H(14C)	0.9800	C(38)-C(39)	1.398(4)
C(15)-H(15A)	0.9800	C(38)-C(43)	1.402(3)
C(15)-H(15B)	0.9800	C(39)-C(40)	1.387(3)
C(15)-H(15C)	0.9800	C(39)-H(39)	0.9500
C(17)-C(18)	1.528(3)	C(40)-C(41)	1.385(4)
C(17)-H(17A)	0.9900	C(40)-H(40)	0.9500
C(17)-H(17B)	0.9900	C(41)-C(42)	1.379(4)
C(18)-H(18A)	0.9900	C(41)-H(41)	0.9500
C(18)-H(18B)	0.9900	C(42)-C(43)	1.395(4)
C(19)-C(20)	1.396(3)	C(42)-H(42)	0.9500
C(19)-C(24)	1.399(3)	C(43)-H(43)	0.9500
C(20)-C(21)	1.391(3)		

C(37)-Ru(1)-C(16)	98.28(9)	C(8)-C(13)-C(15)	120.8(2)
C(37)-Ru(1)-O(1)	98.70(9)	C(9)-C(14)-H(14A)	109.5
C(16)-Ru(1)-O(1)	83.79(7)	C(9)-C(14)-H(14B)	109.5
C(37)-Ru(1)-N(1)	103.07(8)	H(14A)-C(14)-H(14B)	109.5
C(16)-Ru(1)-N(1)	158.34(8)	C(9)-C(14)-H(14C)	109.5
O(1)-Ru(1)-N(1)	89.40(6)	H(14A)-C(14)-H(14C)	109.5
C(37)-Ru(1)-Cl(1)	88.79(8)	H(14B)-C(14)-H(14C)	109.5
C(16)-Ru(1)-Cl(1)	94.73(6)	C(13)-C(15)-H(15A)	109.5
O(1)-Ru(1)-Cl(1)	172.50(4)	C(13)-C(15)-H(15B)	109.5
N(1)-Ru(1)-Cl(1)	89.35(5)	H(15A)-C(15)-H(15B)	109.5
C(1)-O(1)-Ru(1)	128.81(14)	C(13)-C(15)-H(15C)	109.5
C(7)-N(1)-C(8)	113.62(18)	H(15A)-C(15)-H(15C)	109.5
C(7)-N(1)-Ru(1)	123.27(15)	H(15B)-C(15)-H(15C)	109.5
C(8)-N(1)-Ru(1)	122.74(14)	N(3)-C(16)-N(2)	107.30(18)
C(16)-N(2)-C(28)	126.34(18)	N(3)-C(16)-Ru(1)	132.79(16)
C(16)-N(2)-C(18)	113.45(18)	N(2)-C(16)-Ru(1)	119.09(15)
C(28)-N(2)-C(18)	120.19(17)	N(3)-C(17)-C(18)	102.23(17)
C(16)-N(3)-C(19)	126.97(18)	N(3)-C(17)-H(17A)	111.3
C(16)-N(3)-C(17)	113.04(18)	C(18)-C(17)-H(17A)	111.3
C(19)-N(3)-C(17)	119.04(17)	N(3)-C(17)-H(17B)	111.3
O(1)-C(1)-C(2)	117.95(19)	C(18)-C(17)-H(17B)	111.3
O(1)-C(1)-C(6)	124.8(2)	H(17A)-C(17)-H(17B)	109.2
C(2)-C(1)-C(6)	117.2(2)	N(2)-C(18)-C(17)	101.67(17)
C(3)-C(2)-C(1)	121.8(2)	N(2)-C(18)-H(18A)	111.4
C(3)-C(2)-H(2)	119.1	C(17)-C(18)-H(18A)	111.4
C(1)-C(2)-H(2)	119.1	N(2)-C(18)-H(18B)	111.4
C(2)-C(3)-C(4)	121.2(2)	C(17)-C(18)-H(18B)	111.4
C(2)-C(3)-H(3)	119.4	H(18A)-C(18)-H(18B)	109.3
C(4)-C(3)-H(3)	119.4	C(20)-C(19)-C(24)	121.9(2)
C(5)-C(4)-C(3)	118.2(2)	C(20)-C(19)-N(3)	118.9(2)
C(5)-C(4)-H(4)	120.9	C(24)-C(19)-N(3)	119.2(2)
C(3)-C(4)-H(4)	120.9	C(21)-C(20)-C(19)	118.0(2)
C(4)-C(5)-C(6)	122.6(2)	C(21)-C(20)-C(25)	120.5(2)
C(4)-C(5)-H(5)	118.7	C(19)-C(20)-C(25)	121.5(2)
C(6)-C(5)-H(5)	118.7	C(22)-C(21)-C(20)	121.9(2)
C(5)-C(6)-C(7)	117.2(2)	C(22)-C(21)-H(21)	119.0
C(5)-C(6)-C(1)	119.0(2)	C(20)-C(21)-H(21)	119.0
C(7)-C(6)-C(1)	123.8(2)	C(23)-C(22)-C(21)	118.6(2)
N(1)-C(7)-C(6)	129.6(2)	C(23)-C(22)-C(26)	120.7(2)
N(1)-C(7)-H(7)	115.2	C(21)-C(22)-C(26)	120.8(2)
C(6)-C(7)-H(7)	115.2	C(22)-C(23)-C(24)	121.8(2)
C(9)-C(8)-C(13)	121.8(2)	C(22)-C(23)-H(23)	119.1
C(9)-C(8)-N(1)	120.70(19)	C(24)-C(23)-H(23)	119.1
C(13)-C(8)-N(1)	117.49(19)	C(23)-C(24)-C(19)	117.8(2)
C(10)-C(9)-C(8)	118.3(2)	C(23)-C(24)-C(27)	120.5(2)
C(10)-C(9)-C(14)	120.1(2)	C(19)-C(24)-C(27)	121.7(2)
C(8)-C(9)-C(14)	121.6(2)	C(20)-C(25)-H(25A)	109.5
C(11)-C(10)-C(9)	119.6(2)	C(20)-C(25)-H(25B)	109.5
C(11)-C(10)-H(10)	120.2	H(25A)-C(25)-H(25B)	109.5
C(9)-C(10)-H(10)	120.2	C(20)-C(25)-H(25C)	109.5
C(12)-C(11)-C(10)	122.3(2)	H(25A)-C(25)-H(25C)	109.5
C(12)-C(11)-Br(1)	117.85(17)	H(25B)-C(25)-H(25C)	109.5
C(10)-C(11)-Br(1)	119.80(17)	C(22)-C(26)-H(26A)	109.5
C(11)-C(12)-C(13)	119.3(2)	C(22)-C(26)-H(26B)	109.5
C(11)-C(12)-H(12)	120.4	H(26A)-C(26)-H(26B)	109.5
C(13)-C(12)-H(12)	120.4	C(22)-C(26)-H(26C)	109.5
C(12)-C(13)-C(8)	118.7(2)	H(26A)-C(26)-H(26C)	109.5
C(12)-C(13)-C(15)	120.5(2)	H(26B)-C(26)-H(26C)	109.5

C(24)-C(27)-H(27A)	109.5	H(35A)-C(35)-H(35B)	109.5
C(24)-C(27)-H(27B)	109.5	C(31)-C(35)-H(35C)	109.5
H(27A)-C(27)-H(27B)	109.5	H(35A)-C(35)-H(35C)	109.5
C(24)-C(27)-H(27C)	109.5	H(35B)-C(35)-H(35C)	109.5
H(27A)-C(27)-H(27C)	109.5	C(33)-C(36)-H(36A)	109.5
H(27B)-C(27)-H(27C)	109.5	C(33)-C(36)-H(36B)	109.5
C(33)-C(28)-C(29)	121.4(2)	H(36A)-C(36)-H(36B)	109.5
C(33)-C(28)-N(2)	119.8(2)	C(33)-C(36)-H(36C)	109.5
C(29)-C(28)-N(2)	118.6(2)	H(36A)-C(36)-H(36C)	109.5
C(30)-C(29)-C(28)	118.0(2)	H(36B)-C(36)-H(36C)	109.5
C(30)-C(29)-C(34)	119.8(2)	C(38)-C(37)-Ru(1)	134.46(18)
C(28)-C(29)-C(34)	122.2(2)	C(38)-C(37)-H(37)	112.8
C(31)-C(30)-C(29)	122.2(2)	Ru(1)-C(37)-H(37)	112.8
C(31)-C(30)-H(30)	118.9	C(39)-C(38)-C(43)	118.1(2)
C(29)-C(30)-H(30)	118.9	C(39)-C(38)-C(37)	125.3(2)
C(32)-C(31)-C(30)	118.5(2)	C(43)-C(38)-C(37)	116.6(2)
C(32)-C(31)-C(35)	121.4(2)	C(40)-C(39)-C(38)	120.9(2)
C(30)-C(31)-C(35)	120.1(2)	C(40)-C(39)-H(39)	119.5
C(31)-C(32)-C(33)	121.9(2)	C(38)-C(39)-H(39)	119.5
C(31)-C(32)-H(32)	119.0	C(41)-C(40)-C(39)	120.2(3)
C(33)-C(32)-H(32)	119.0	C(41)-C(40)-H(40)	119.9
C(28)-C(33)-C(32)	117.9(2)	C(39)-C(40)-H(40)	119.9
C(28)-C(33)-C(36)	122.4(2)	C(42)-C(41)-C(40)	119.9(3)
C(32)-C(33)-C(36)	119.6(2)	C(42)-C(41)-H(41)	120.0
C(29)-C(34)-H(34A)	109.5	C(40)-C(41)-H(41)	120.0
C(29)-C(34)-H(34B)	109.5	C(41)-C(42)-C(43)	120.1(3)
H(34A)-C(34)-H(34B)	109.5	C(41)-C(42)-H(42)	119.9
C(29)-C(34)-H(34C)	109.5	C(43)-C(42)-H(42)	119.9
H(34A)-C(34)-H(34C)	109.5	C(42)-C(43)-C(38)	120.7(3)
H(34B)-C(34)-H(34C)	109.5	C(42)-C(43)-H(43)	119.7
C(31)-C(35)-H(35A)	109.5	C(38)-C(43)-H(43)	119.7
C(31)-C(35)-H(35B)	109.5		

Symmetry transformations were used to generate equivalent atoms.

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) of complex **7a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\, a^{*2} U^{11} + \ldots + 2\, h\, k\, a^*\, b^*\, U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	14(1)	10(1)	15(1)	2(1)	2(1)	4(1)
Br(1)	26(1)	17(1)	29(1)	7(1)	8(1)	-1(1)
Cl(1)	25(1)	16(1)	21(1)	7(1)	2(1)	3(1)
O(1)	16(1)	13(1)	17(1)	4(1)	2(1)	3(1)
N(1)	15(1)	12(1)	18(1)	3(1)	3(1)	5(1)
N(2)	15(1)	12(1)	20(1)	1(1)	1(1)	4(1)
N(3)	16(1)	14(1)	18(1)	1(1)	1(1)	6(1)
C(1)	17(1)	15(1)	18(1)	3(1)	3(1)	10(1)
C(2)	19(1)	14(1)	25(1)	6(1)	3(1)	6(1)
C(3)	21(1)	20(1)	26(1)	13(1)	8(1)	8(1)
C(4)	25(1)	21(1)	18(1)	6(1)	3(1)	11(1)
C(5)	22(1)	14(1)	18(1)	1(1)	1(1)	7(1)
C(6)	17(1)	14(1)	19(1)	4(1)	4(1)	9(1)
C(7)	16(1)	13(1)	20(1)	1(1)	2(1)	7(1)
C(8)	17(1)	12(1)	15(1)	2(1)	-1(1)	2(1)
C(9)	17(1)	18(1)	15(1)	5(1)	1(1)	6(1)
C(10)	16(1)	21(1)	17(1)	6(1)	5(1)	6(1)
C(11)	20(1)	13(1)	17(1)	4(1)	1(1)	-2(1)
C(12)	21(1)	12(1)	19(1)	2(1)	2(1)	5(1)
C(13)	16(1)	16(1)	18(1)	3(1)	2(1)	5(1)
C(14)	22(1)	18(1)	25(1)	8(1)	6(1)	8(1)
C(15)	19(1)	16(1)	29(1)	2(1)	4(1)	7(1)
C(16)	20(1)	11(1)	15(1)	5(1)	1(1)	6(1)
C(17)	18(1)	19(1)	25(1)	1(1)	-3(1)	7(1)
C(18)	16(1)	16(1)	22(1)	2(1)	-1(1)	5(1)
C(19)	18(1)	13(1)	14(1)	-1(1)	-1(1)	5(1)
C(20)	19(1)	14(1)	17(1)	3(1)	-1(1)	4(1)
C(21)	23(1)	12(1)	22(1)	2(1)	1(1)	7(1)
C(22)	22(1)	18(1)	19(1)	2(1)	2(1)	8(1)
C(23)	24(1)	21(1)	16(1)	5(1)	4(1)	6(1)
C(24)	20(1)	15(1)	17(1)	4(1)	-2(1)	4(1)
C(25)	29(1)	22(1)	22(1)	8(1)	7(1)	11(1)
C(26)	33(1)	22(1)	29(1)	6(1)	10(1)	14(1)
C(27)	30(1)	19(1)	21(1)	7(1)	1(1)	8(1)
C(28)	15(1)	14(1)	21(1)	2(1)	2(1)	6(1)
C(29)	17(1)	19(1)	22(1)	6(1)	2(1)	8(1)
C(30)	20(1)	14(1)	26(1)	8(1)	4(1)	7(1)
C(31)	16(1)	15(1)	25(1)	3(1)	4(1)	7(1)
C(32)	19(1)	19(1)	19(1)	4(1)	5(1)	9(1)
C(33)	15(1)	16(1)	23(1)	6(1)	5(1)	7(1)
C(34)	33(1)	23(1)	21(1)	7(1)	2(1)	13(1)
C(35)	29(1)	15(1)	31(1)	3(1)	6(1)	8(1)
C(36)	29(1)	20(1)	26(1)	9(1)	11(1)	12(1)
C(37)	17(1)	16(1)	18(1)	1(1)	0(1)	4(1)
C(38)	18(1)	17(1)	22(1)	-1(1)	-1(1)	7(1)
C(39)	26(1)	19(1)	21(1)	1(1)	0(1)	11(1)
C(40)	37(1)	24(1)	28(1)	6(1)	1(1)	16(1)
C(41)	43(2)	33(2)	47(2)	9(1)	7(1)	29(1)
C(42)	42(2)	38(2)	52(2)	11(1)	20(1)	30(1)
C(43)	27(1)	28(1)	37(2)	8(1)	11(1)	14(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) of complex **7a**.

	x	*y*	*z*	*U*(eq)
H(2)	8404	11745	831	23
H(3)	7878	11410	-600	25
H(4)	6137	9521	-1435	25
H(5)	4916	8044	-777	23
H(7)	4426	7283	366	20
H(10)	1377	5477	2134	22
H(12)	3709	3528	1223	22
H(14A)	3345	8493	2783	32
H(14B)	1933	7738	2271	32
H(14C)	3094	8435	1805	32
H(15A)	5797	4637	970	33
H(15B)	6451	6144	1573	33
H(15C)	5922	5813	588	33
H(17A)	10693	11489	4507	27
H(17B)	11020	12464	3927	27
H(18A)	11171	10875	2769	23
H(18B)	11220	10073	3427	23
H(21)	8191	14893	4604	23
H(23)	6924	12295	5920	25
H(25A)	9099	14369	3314	35
H(25B)	9095	12908	2905	35
H(25C)	10265	14021	3590	35
H(26A)	6128	14027	6146	41
H(26B)	6403	14906	5513	41
H(26C)	7422	15301	6329	41
H(27A)	7523	10452	5676	35
H(27B)	8663	10383	5113	35
H(27C)	7215	9693	4661	35
H(30)	8694	5269	2203	23
H(32)	9060	6731	219	22
H(34A)	8254	6660	3609	37
H(34B)	8901	8233	3829	37
H(34C)	9777	7379	3761	37
H(35A)	8468	4423	-91	39
H(35B)	7807	3788	621	39
H(35C)	9310	4175	585	39
H(36A)	9307	9957	1400	35
H(36B)	9132	8967	444	35
H(36C)	10499	9642	1017	35
H(37)	5703	9930	3708	22
H(39)	6739	11903	2269	27
H(40)	6218	13727	2332	35
H(41)	4833	14287	3283	46
H(42)	4020	13063	4206	48
H(43)	4571	11256	4173	36

Table S6. Torsion angles [°] of complex **7a**.

C(37)-Ru(1)-O(1)-C(1)	-108.13(18)	C(18)-N(2)-C(16)-Ru(1)	164.69(15)
C(16)-Ru(1)-O(1)-C(1)	154.40(18)	C(37)-Ru(1)-C(16)-N(3)	-15.3(2)
N(1)-Ru(1)-O(1)-C(1)	-5.00(17)	O(1)-Ru(1)-C(16)-N(3)	82.6(2)
Cl(1)-Ru(1)-O(1)-C(1)	75.4(4)	N(1)-Ru(1)-C(16)-N(3)	154.99(19)
C(37)-Ru(1)-N(1)-C(7)	104.10(18)	Cl(1)-Ru(1)-C(16)-N(3)	-104.8(2)
C(16)-Ru(1)-N(1)-C(7)	-66.1(3)	C(37)-Ru(1)-C(16)-N(2)	176.52(17)
O(1)-Ru(1)-N(1)-C(7)	5.31(17)	O(1)-Ru(1)-C(16)-N(2)	-85.55(17)
Cl(1)-Ru(1)-N(1)-C(7)	-167.29(17)	N(1)-Ru(1)-C(16)-N(2)	-13.2(3)
C(37)-Ru(1)-N(1)-C(8)	-83.25(17)	Cl(1)-Ru(1)-C(16)-N(2)	87.06(16)
C(16)-Ru(1)-N(1)-C(8)	106.6(2)	C(16)-N(3)-C(17)-C(18)	12.4(3)
O(1)-Ru(1)-N(1)-C(8)	177.96(16)	C(19)-N(3)-C(17)-C(18)	-178.00(19)
Cl(1)-Ru(1)-N(1)-C(8)	5.35(15)	C(16)-N(2)-C(18)-C(17)	13.4(2)
Ru(1)-O(1)-C(1)-C(2)	-177.19(14)	C(28)-N(2)-C(18)-C(17)	-167.92(19)
Ru(1)-O(1)-C(1)-C(6)	2.2(3)	N(3)-C(17)-C(18)-N(2)	-14.2(2)
O(1)-C(1)-C(2)-C(3)	176.9(2)	C(16)-N(3)-C(19)-C(20)	-110.3(3)
C(6)-C(1)-C(2)-C(3)	-2.5(3)	C(17)-N(3)-C(19)-C(20)	81.6(3)
C(1)-C(2)-C(3)-C(4)	0.8(4)	C(16)-N(3)-C(19)-C(24)	72.1(3)
C(2)-C(3)-C(4)-C(5)	1.3(3)	C(17)-N(3)-C(19)-C(24)	-95.9(3)
C(3)-C(4)-C(5)-C(6)	-1.8(3)	C(24)-C(19)-C(20)-C(21)	-1.8(3)
C(4)-C(5)-C(6)-C(7)	-179.7(2)	N(3)-C(19)-C(20)-C(21)	-179.28(19)
C(4)-C(5)-C(6)-C(1)	0.1(3)	C(24)-C(19)-C(20)-C(25)	179.8(2)
O(1)-C(1)-C(6)-C(5)	-177.4(2)	N(3)-C(19)-C(20)-C(25)	2.4(3)
C(2)-C(1)-C(6)-C(5)	2.0(3)	C(19)-C(20)-C(21)-C(22)	-0.6(3)
O(1)-C(1)-C(6)-C(7)	2.5(3)	C(25)-C(20)-C(21)-C(22)	177.8(2)
C(2)-C(1)-C(6)-C(7)	-178.2(2)	C(20)-C(21)-C(22)-C(23)	2.1(3)
C(8)-N(1)-C(7)-C(6)	-176.5(2)	C(20)-C(21)-C(22)-C(26)	-176.6(2)
Ru(1)-N(1)-C(7)-C(6)	-3.3(3)	C(21)-C(22)-C(23)-C(24)	-1.2(3)
C(5)-C(6)-C(7)-N(1)	178.1(2)	C(26)-C(22)-C(23)-C(24)	177.5(2)
C(1)-C(6)-C(7)-N(1)	-1.7(4)	C(22)-C(23)-C(24)-C(19)	-1.1(3)
C(7)-N(1)-C(8)-C(9)	-93.8(2)	C(22)-C(23)-C(24)-C(27)	179.8(2)
Ru(1)-N(1)-C(8)-C(9)	92.9(2)	C(20)-C(19)-C(24)-C(23)	2.7(3)
C(7)-N(1)-C(8)-C(13)	84.8(2)	N(3)-C(19)-C(24)-C(23)	-179.90(19)
Ru(1)-N(1)-C(8)-C(13)	-88.5(2)	C(20)-C(19)-C(24)-C(27)	-178.3(2)
C(13)-C(8)-C(9)-C(10)	-2.0(3)	N(3)-C(19)-C(24)-C(27)	-0.8(3)
N(1)-C(8)-C(9)-C(10)	176.53(19)	C(16)-N(2)-C(28)-C(33)	95.2(3)
C(13)-C(8)-C(9)-C(14)	177.0(2)	C(18)-N(2)-C(28)-C(33)	-83.2(3)
N(1)-C(8)-C(9)-C(14)	-4.5(3)	C(16)-N(2)-C(28)-C(29)	-90.2(3)
C(8)-C(9)-C(10)-C(11)	0.3(3)	C(18)-N(2)-C(28)-C(29)	91.3(3)
C(14)-C(9)-C(10)-C(11)	-178.7(2)	C(33)-C(28)-C(29)-C(30)	-2.9(3)
C(9)-C(10)-C(11)-C(12)	1.4(3)	N(2)-C(28)-C(29)-C(30)	-177.35(19)
C(9)-C(10)-C(11)-Br(1)	-178.10(16)	C(33)-C(28)-C(29)-C(34)	176.6(2)
C(10)-C(11)-C(12)-C(13)	-1.3(3)	N(2)-C(28)-C(29)-C(34)	2.2(3)
Br(1)-C(11)-C(12)-C(13)	178.16(16)	C(28)-C(29)-C(30)-C(31)	0.0(3)
C(11)-C(12)-C(13)-C(8)	-0.4(3)	C(34)-C(29)-C(30)-C(31)	-179.6(2)
C(11)-C(12)-C(13)-C(15)	177.3(2)	C(29)-C(30)-C(31)-C(32)	1.7(3)
C(9)-C(8)-C(13)-C(12)	2.0(3)	C(29)-C(30)-C(31)-C(35)	-177.3(2)
N(1)-C(8)-C(13)-C(12)	-176.52(19)	C(30)-C(31)-C(32)-C(33)	-0.5(3)
C(9)-C(8)-C(13)-C(15)	-175.6(2)	C(35)-C(31)-C(32)-C(33)	178.5(2)
N(1)-C(8)-C(13)-C(15)	5.8(3)	C(29)-C(28)-C(33)-C(32)	4.1(3)
C(19)-N(3)-C(16)-N(2)	-173.1(2)	N(2)-C(28)-C(33)-C(32)	178.42(19)
C(17)-N(3)-C(16)-N(2)	-4.4(3)	C(29)-C(28)-C(33)-C(36)	-173.7(2)
C(19)-N(3)-C(16)-Ru(1)	17.8(3)	N(2)-C(28)-C(33)-C(36)	0.7(3)
C(17)-N(3)-C(16)-Ru(1)	-173.61(17)	C(31)-C(32)-C(33)-C(28)	-2.3(3)
C(28)-N(2)-C(16)-N(3)	175.2(2)	C(31)-C(32)-C(33)-C(36)	175.5(2)
C(18)-N(2)-C(16)-N(3)	-6.2(3)	C(16)-Ru(1)-C(37)-C(38)	95.1(2)
C(28)-N(2)-C(16)-Ru(1)	-13.8(3)	O(1)-Ru(1)-C(37)-C(38)	10.1(2)

N(1)-Ru(1)-C(37)-C(38)	-81.3(2)
Cl(1)-Ru(1)-C(37)-C(38)	-170.3(2)
Ru(1)-C(37)-C(38)-C(39)	-12.3(4)
Ru(1)-C(37)-C(38)-C(43)	168.22(19)
C(43)-C(38)-C(39)-C(40)	-0.6(3)
C(37)-C(38)-C(39)-C(40)	179.9(2)
C(38)-C(39)-C(40)-C(41)	-0.6(4)
C(39)-C(40)-C(41)-C(42)	1.2(4)
C(40)-C(41)-C(42)-C(43)	-0.4(5)
C(41)-C(42)-C(43)-C(38)	-0.9(5)
C(39)-C(38)-C(43)-C(42)	1.4(4)
C(37)-C(38)-C(43)-C(42)	-179.1(2)

Symmetry transformations were used to generate equivalent atoms.