Synthesis and Catalytic Activity of Water-soluble Ruthenium(II) Complexes Bearing Naphthyridine-Carboxylate Ligands

*Chang-Yao Huang, Kai-Yuan Kuan, Yi-Hong Liu, Shie-Ming Peng and Shiuh-Tzung Liu**

Department of Chemistry, National Taiwan University, Taipei 106, Taiwan

Supplementary Materials (18 pages)

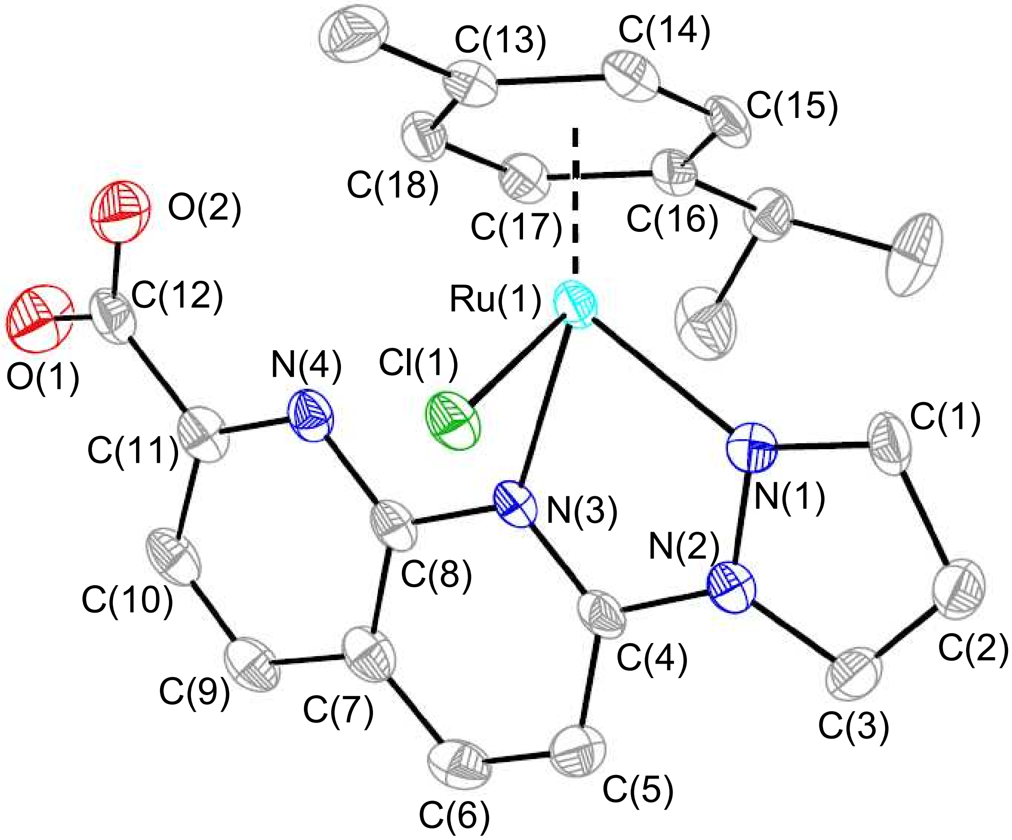

Figure S1 ORTEP plot of **6** (Drawn with 30 % probability ellipsoids)

Table S0 Crystal data for **5** and **6**

Complex	**5**·H_2O	**6**·$(CH_3OH)_3$
Formula	$C_{18}H_{14}Cl_2N_4O_2Ru \cdot H_2O$	$C_{22}H_{22}Cl_2N_4O_2Ru \cdot (CH_3OH)_3$
Fw	508.32	630.44
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a, Å	11.3420(2)	7.8960(4)
b, Å	11.6987(3)	13.1226(8)
c, Å	15.0966(3)	13.8467(7)
α, deg	106.978(2)	83.174(5)
β, deg	94.433(2)	85.479(4)
γ, deg	101.557(2)	79.467(5)
V, $Å^3$; Z	1857.16(7), 4	1398.17(13), 2
d (calc.), Mg/m^3	1.818	1.497
F(0,0,0)	1016	636
Crystal size, mm^3	0.20 x 0.15 x 0.10	0.25 x 0.20 x 0.10
Rflns collected	40195	13430
Independent rflns	8417 [R(int) = 0.0315]	6220 [R(int) = 0.0726]
θ range, deg	2.87 to 27.50°	2.94 to 27.50°
Refined method	Full-matrix least-squares on F^2	
Goodness of fit on F^2	1.062	1.002
R indices [$I>2\sigma(I)$]	R1 = 0.0372, wR2 = 0.0993	R1 = 0.0715, wR2 = 0.1965
R indices (all data)	R1 = 0.0455, wR2 = 0.1046	R1 = 0.0881, wR2 = 0.2193

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for complex **5 (**ic16099). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	6821(1)	7177(1)	3491(1)	15(1)
Cl(1)	5739(1)	8216(1)	4660(1)	19(1)
O(1)	6250(4)	9163(3)	1051(3)	37(1)
O(2)	4480(4)	9282(3)	368(3)	39(1)
N(1)	6343(3)	5680(3)	3952(2)	17(1)
N(2)	5178(3)	5007(3)	3653(2)	16(1)
N(3)	5026(3)	6285(3)	2779(2)	16(1)
N(4)	4998(3)	7541(3)	1845(2)	20(1)
C(1)	6865(4)	5115(4)	4462(3)	21(1)
C(2)	6039(4)	4062(4)	4484(3)	22(1)
C(3)	4975(4)	4018(4)	3978(3)	20(1)
C(4)	4442(4)	5386(4)	3065(3)	17(1)
C(5)	3193(4)	4831(4)	2824(3)	24(1)
C(6)	2532(4)	5232(4)	2235(3)	27(1)
C(7)	3110(4)	6146(4)	1871(3)	24(1)
C(8)	4370(4)	6671(4)	2157(3)	18(1)
C(9)	2510(5)	6568(5)	1215(3)	31(1)
C(10)	3155(5)	7415(5)	887(3)	31(1)
C(11)	4407(5)	7894(4)	1224(3)	25(1)
C(12)	5148(5)	8864(4)	865(3)	29(1)
C(13)	8200(4)	6561(5)	2672(4)	34(1)
C(14)	8701(4)	7076(5)	3631(4)	36(1)
C(15)	8630(4)	8265(5)	4142(4)	33(1)
C(16)	8077(4)	8959(5)	3682(4)	30(1)
C(17)	7581(4)	8471(5)	2747(4)	28(1)
C(18)	7610(4)	7257(5)	2241(3)	31(1)
Ru(2)	1719(1)	10634(1)	2038(1)	15(1)
Cl(2)	1881(1)	12122(1)	3554(1)	22(1)
O(3)	3427(3)	13553(3)	461(3)	33(1)
O(4)	5346(3)	14525(3)	528(3)	34(1)

N(5)	1900(3)	9444(3)	2780(3)	19(1)
N(6)	3052(3)	9520(3)	3162(2)	16(1)
N(7)	3642(3)	10898(3)	2383(2)	15(1)
N(8)	4153(3)	12304(3)	1595(2)	17(1)
C(19)	1179(4)	8658(5)	3086(4)	28(1)
C(20)	1859(4)	8216(4)	3668(4)	28(1)
C(21)	3037(4)	8778(4)	3712(3)	22(1)
C(22)	4000(4)	10299(4)	2936(3)	15(1)
C(23)	5212(4)	10375(4)	3277(3)	18(1)
C(24)	6102(4)	11107(4)	3002(3)	19(1)
C(25)	5783(4)	11771(4)	2410(3)	17(1)
C(26)	4541(4)	11669(4)	2120(3)	15(1)
C(27)	6647(4)	12557(4)	2099(3)	23(1)
C(28)	6275(4)	13180(4)	1579(3)	25(1)
C(29)	4988(4)	13049(4)	1326(3)	19(1)
C(30)	4520(4)	13752(4)	723(3)	23(1)
C(31)	1457(5)	11567(6)	991(4)	44(2)
C(32)	484(5)	11574(5)	1496(4)	39(1)
C(33)	-192(4)	10488(6)	1581(4)	35(1)
C(34)	98(5)	9380(5)	1148(4)	37(1)
C(35)	1072(5)	9340(5)	631(4)	42(2)
C(36)	1773(5)	10446(8)	570(4)	49(2)
Cl(3)	642(2)	5887(2)	-997(2)	71(1)
Cl(4)	-1150(4)	6287(4)	356(3)	48(1)
Cl(4')	862(2)	15807(2)	4590(2)	44(1)
O(5)	9059(5)	11951(8)	3782(7)	131(4)
O(6)	-417(8)	14157(11)	2805(8)	161(5)

Table S2. Bond lengths [Å] and angles [°] for complex **5 (**ic16099).

Ru(1)-N(1)	2.057(4)	C(17)-C(18)	1.411(7)
Ru(1)-N(3)	2.132(3)	Ru(2)-N(5)	2.054(4)
Ru(1)-C(14)	2.156(5)	Ru(2)-N(7)	2.141(3)
Ru(1)-C(18)	2.169(5)	Ru(2)-C(36)	2.170(5)
Ru(1)-C(15)	2.169(5)	Ru(2)-C(34)	2.173(5)
Ru(1)-C(13)	2.174(5)	Ru(2)-C(33)	2.181(5)
Ru(1)-C(16)	2.204(5)	Ru(2)-C(35)	2.185(5)
Ru(1)-C(17)	2.219(4)	Ru(2)-C(32)	2.193(5)
Ru(1)-Cl(1)	2.4030(10)	Ru(2)-C(31)	2.201(5)
O(1)-C(12)	1.215(7)	Ru(2)-Cl(2)	2.4054(11)
O(2)-C(12)	1.286(6)	O(3)-C(30)	1.226(6)
N(1)-C(1)	1.328(5)	O(4)-C(30)	1.281(6)
N(1)-N(2)	1.361(5)	N(5)-C(19)	1.317(6)
N(2)-C(3)	1.369(5)	N(5)-N(6)	1.363(5)
N(2)-C(4)	1.395(5)	N(6)-C(21)	1.364(5)
N(3)-C(4)	1.327(5)	N(6)-C(22)	1.396(5)
N(3)-C(8)	1.384(5)	N(7)-C(22)	1.324(5)
N(4)-C(11)	1.319(6)	N(7)-C(26)	1.384(5)
N(4)-C(8)	1.344(6)	N(8)-C(29)	1.326(5)
C(1)-C(2)	1.401(6)	N(8)-C(26)	1.339(5)
C(2)-C(3)	1.361(6)	C(19)-C(20)	1.398(7)
C(4)-C(5)	1.405(6)	C(20)-C(21)	1.353(6)
C(5)-C(6)	1.361(7)	C(22)-C(23)	1.406(6)
C(6)-C(7)	1.411(7)	C(23)-C(24)	1.360(6)
C(7)-C(8)	1.415(6)	C(24)-C(25)	1.415(6)
C(7)-C(9)	1.416(7)	C(25)-C(27)	1.410(6)
C(9)-C(10)	1.348(8)	C(25)-C(26)	1.413(6)
C(10)-C(11)	1.411(7)	C(27)-C(28)	1.317(7)
C(11)-C(12)	1.528(7)	C(28)-C(29)	1.446(6)
C(13)-C(18)	1.412(8)	C(29)-C(30)	1.523(6)
C(13)-C(14)	1.417(8)	C(31)-C(32)	1.389(9)
C(14)-C(15)	1.401(8)	C(31)-C(36)	1.411(10)
C(15)-C(16)	1.415(8)	C(32)-C(33)	1.393(8)
C(16)-C(17)	1.384(7)	C(33)-C(34)	1.387(8)

C(34)-C(35)	1.401(9)	C(35)-C(36)	1.408(10)
N(1)-Ru(1)-N(3)	75.71(13)	C(16)-Ru(1)-Cl(1)	88.72(14)
N(1)-Ru(1)-C(14)	90.55(16)	C(17)-Ru(1)-Cl(1)	107.95(14)
N(3)-Ru(1)-C(14)	145.97(19)	C(1)-N(1)-N(2)	106.1(3)
N(1)-Ru(1)-C(18)	128.04(18)	C(1)-N(1)-Ru(1)	138.2(3)
N(3)-Ru(1)-C(18)	95.40(16)	N(2)-N(1)-Ru(1)	115.7(3)
C(14)-Ru(1)-C(18)	68.6(2)	N(1)-N(2)-C(3)	110.6(3)
N(1)-Ru(1)-C(15)	111.36(17)	N(1)-N(2)-C(4)	117.4(3)
N(3)-Ru(1)-C(15)	172.88(17)	C(3)-N(2)-C(4)	132.0(4)
C(14)-Ru(1)-C(15)	37.8(2)	C(4)-N(3)-C(8)	117.7(4)
C(18)-Ru(1)-C(15)	80.94(19)	C(4)-N(3)-Ru(1)	115.7(3)
N(1)-Ru(1)-C(13)	97.68(17)	C(8)-N(3)-Ru(1)	125.9(3)
N(3)-Ru(1)-C(13)	112.02(18)	C(11)-N(4)-C(8)	117.8(4)
C(14)-Ru(1)-C(13)	38.2(2)	N(1)-C(1)-C(2)	110.2(4)
C(18)-Ru(1)-C(13)	37.9(2)	C(3)-C(2)-C(1)	106.4(4)
C(15)-Ru(1)-C(13)	68.7(2)	C(2)-C(3)-N(2)	106.7(4)
N(1)-Ru(1)-C(16)	147.85(18)	N(3)-C(4)-N(2)	114.2(4)
N(3)-Ru(1)-C(16)	135.15(17)	N(3)-C(4)-C(5)	125.3(4)
C(14)-Ru(1)-C(16)	67.7(2)	N(2)-C(4)-C(5)	120.5(4)
C(18)-Ru(1)-C(16)	67.2(2)	C(6)-C(5)-C(4)	117.4(4)
C(15)-Ru(1)-C(16)	37.8(2)	C(5)-C(6)-C(7)	120.0(4)
C(13)-Ru(1)-C(16)	79.96(19)	C(6)-C(7)-C(8)	119.2(4)
N(1)-Ru(1)-C(17)	165.05(17)	C(6)-C(7)-C(9)	123.9(4)
N(3)-Ru(1)-C(17)	105.98(16)	C(8)-C(7)-C(9)	116.9(5)
C(14)-Ru(1)-C(17)	79.94(18)	N(4)-C(8)-N(3)	116.3(4)
C(18)-Ru(1)-C(17)	37.5(2)	N(4)-C(8)-C(7)	123.4(4)
C(15)-Ru(1)-C(17)	67.44(19)	N(3)-C(8)-C(7)	120.3(4)
C(13)-Ru(1)-C(17)	67.74(19)	C(10)-C(9)-C(7)	119.3(5)
C(16)-Ru(1)-C(17)	36.5(2)	C(9)-C(10)-C(11)	119.6(4)
N(1)-Ru(1)-Cl(1)	86.99(10)	N(4)-C(11)-C(10)	123.1(5)
N(3)-Ru(1)-Cl(1)	82.50(9)	N(4)-C(11)-C(12)	116.7(4)
C(14)-Ru(1)-Cl(1)	128.43(17)	C(10)-C(11)-C(12)	120.2(4)
C(18)-Ru(1)-Cl(1)	143.47(15)	O(1)-C(12)-O(2)	126.6(5)
C(15)-Ru(1)-Cl(1)	96.77(15)	O(1)-C(12)-C(11)	120.7(4)
C(13)-Ru(1)-Cl(1)	165.42(15)	O(2)-C(12)-C(11)	112.7(5)

C(18)-C(13)-C(14)	118.9(5)	C(34)-Ru(2)-C(32)	66.8(2)
C(18)-C(13)-Ru(1)	70.8(3)	C(33)-Ru(2)-C(32)	37.1(2)
C(14)-C(13)-Ru(1)	70.2(3)	C(35)-Ru(2)-C(32)	79.4(2)
C(15)-C(14)-C(13)	120.7(5)	N(5)-Ru(2)-C(31)	168.2(2)
C(15)-C(14)-Ru(1)	71.6(3)	N(7)-Ru(2)-C(31)	106.51(18)
C(13)-C(14)-Ru(1)	71.6(3)	C(36)-Ru(2)-C(31)	37.7(3)
C(14)-C(15)-C(16)	119.1(5)	C(34)-Ru(2)-C(31)	79.41(19)
C(14)-C(15)-Ru(1)	70.6(3)	C(33)-Ru(2)-C(31)	67.0(2)
C(16)-C(15)-Ru(1)	72.4(3)	C(35)-Ru(2)-C(31)	67.6(2)
C(17)-C(16)-C(15)	121.0(5)	C(32)-Ru(2)-C(31)	36.8(2)
C(17)-C(16)-Ru(1)	72.4(3)	N(5)-Ru(2)-Cl(2)	84.58(11)
C(15)-C(16)-Ru(1)	69.8(3)	N(7)-Ru(2)-Cl(2)	84.47(9)
C(16)-C(17)-C(18)	119.8(5)	C(36)-Ru(2)-Cl(2)	142.9(2)
C(16)-C(17)-Ru(1)	71.2(3)	C(34)-Ru(2)-Cl(2)	128.64(18)
C(18)-C(17)-Ru(1)	69.3(3)	C(33)-Ru(2)-Cl(2)	97.15(15)
C(17)-C(18)-C(13)	120.3(5)	C(35)-Ru(2)-Cl(2)	164.62(15)
C(17)-C(18)-Ru(1)	73.2(3)	C(32)-Ru(2)-Cl(2)	88.10(15)
C(13)-C(18)-Ru(1)	71.2(3)	C(31)-Ru(2)-Cl(2)	107.10(18)
N(5)-Ru(2)-N(7)	75.40(13)	C(19)-N(5)-N(6)	106.0(4)
N(5)-Ru(2)-C(36)	131.2(2)	C(19)-N(5)-Ru(2)	137.4(3)
N(7)-Ru(2)-C(36)	94.88(16)	N(6)-N(5)-Ru(2)	116.2(3)
N(5)-Ru(2)-C(34)	92.29(17)	N(5)-N(6)-C(21)	110.4(3)
N(7)-Ru(2)-C(34)	144.01(19)	N(5)-N(6)-C(22)	117.3(3)
C(36)-Ru(2)-C(34)	67.8(2)	C(21)-N(6)-C(22)	132.3(4)
N(5)-Ru(2)-C(33)	110.95(18)	C(22)-N(7)-C(26)	117.0(3)
N(7)-Ru(2)-C(33)	173.54(18)	C(22)-N(7)-Ru(2)	116.4(3)
C(36)-Ru(2)-C(33)	80.0(2)	C(26)-N(7)-Ru(2)	126.5(3)
C(34)-Ru(2)-C(33)	37.2(2)	C(29)-N(8)-C(26)	117.6(4)
N(5)-Ru(2)-C(35)	100.8(2)	N(5)-C(19)-C(20)	110.4(4)
N(7)-Ru(2)-C(35)	110.79(18)	C(21)-C(20)-C(19)	106.4(4)
C(36)-Ru(2)-C(35)	37.7(3)	C(20)-C(21)-N(6)	106.8(4)
C(34)-Ru(2)-C(35)	37.5(2)	N(7)-C(22)-N(6)	114.3(3)
C(33)-Ru(2)-C(35)	67.5(2)	N(7)-C(22)-C(23)	125.8(4)
N(5)-Ru(2)-C(32)	145.8(2)	N(6)-C(22)-C(23)	119.9(4)
N(7)-Ru(2)-C(32)	137.02(19)	C(24)-C(23)-C(22)	117.5(4)
C(36)-Ru(2)-C(32)	67.3(2)	C(23)-C(24)-C(25)	119.6(4)

C(27)-C(25)-C(26)	117.5(4)	C(36)-C(31)-Ru(2)	70.0(3)
C(27)-C(25)-C(24)	123.2(4)	C(31)-C(32)-C(33)	120.9(5)
C(26)-C(25)-C(24)	119.3(4)	C(31)-C(32)-Ru(2)	71.9(3)
N(8)-C(26)-N(7)	115.8(3)	C(33)-C(32)-Ru(2)	71.0(3)
N(8)-C(26)-C(25)	123.5(4)	C(34)-C(33)-C(32)	119.8(5)
N(7)-C(26)-C(25)	120.7(4)	C(34)-C(33)-Ru(2)	71.1(3)
C(28)-C(27)-C(25)	119.5(4)	C(32)-C(33)-Ru(2)	71.9(3)
C(27)-C(28)-C(29)	119.9(4)	C(33)-C(34)-C(35)	120.8(5)
N(8)-C(29)-C(28)	122.0(4)	C(33)-C(34)-Ru(2)	71.7(3)
N(8)-C(29)-C(30)	116.5(4)	C(35)-C(34)-Ru(2)	71.7(3)
C(28)-C(29)-C(30)	121.6(4)	C(34)-C(35)-C(36)	119.2(5)
O(3)-C(30)-O(4)	125.0(4)	C(34)-C(35)-Ru(2)	70.8(3)
O(3)-C(30)-C(29)	120.1(4)	C(36)-C(35)-Ru(2)	70.5(3)
O(4)-C(30)-C(29)	114.9(4)	C(35)-C(36)-C(31)	119.9(5)
C(32)-C(31)-C(36)	119.4(5)	C(35)-C(36)-Ru(2)	71.7(3)
C(32)-C(31)-Ru(2)	71.3(3)	C(31)-C(36)-Ru(2)	72.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters ($Å^2 x 10^3$) for complex **5** (ic16099). 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)	14(1)	16(1)	16(1)	8(1)	4(1)	4(1)
Cl(1)	20(1)	21(1)	17(1)	5(1)	3(1)	7(1)
O(1)	53(2)	37(2)	32(2)	23(2)	13(2)	17(2)
O(2)	62(3)	35(2)	28(2)	16(2)	-1(2)	24(2)
N(1)	18(2)	17(2)	18(2)	8(1)	2(1)	3(1)
N(2)	18(2)	16(2)	15(2)	5(1)	5(1)	3(1)
N(3)	17(2)	17(2)	13(2)	4(1)	2(1)	5(1)
N(4)	30(2)	19(2)	14(2)	5(1)	3(1)	10(2)
C(1)	25(2)	21(2)	21(2)	10(2)	6(2)	10(2)
C(2)	33(2)	16(2)	20(2)	8(2)	8(2)	11(2)
C(3)	29(2)	15(2)	18(2)	5(2)	9(2)	5(2)
C(4)	21(2)	18(2)	12(2)	4(2)	2(2)	4(2)
C(5)	21(2)	21(2)	25(2)	6(2)	3(2)	0(2)
C(6)	18(2)	30(2)	28(2)	3(2)	-1(2)	2(2)
C(7)	25(2)	24(2)	20(2)	-1(2)	-3(2)	10(2)
C(8)	23(2)	19(2)	12(2)	1(2)	1(2)	10(2)
C(9)	30(2)	31(3)	27(3)	0(2)	-10(2)	13(2)
C(10)	41(3)	31(3)	22(2)	7(2)	-7(2)	21(2)
C(11)	40(3)	23(2)	14(2)	2(2)	4(2)	17(2)
C(12)	55(3)	25(2)	13(2)	7(2)	7(2)	20(2)
C(13)	24(2)	27(3)	54(3)	11(2)	23(2)	7(2)
C(14)	15(2)	47(3)	63(4)	41(3)	13(2)	10(2)
C(15)	17(2)	48(3)	31(3)	18(2)	2(2)	-8(2)
C(16)	24(2)	23(2)	43(3)	11(2)	14(2)	-2(2)
C(17)	22(2)	33(3)	40(3)	28(2)	12(2)	6(2)
C(18)	24(2)	46(3)	23(2)	10(2)	14(2)	3(2)
Ru(2)	13(1)	17(1)	15(1)	7(1)	-1(1)	2(1)
Cl(2)	19(1)	26(1)	18(1)	4(1)	2(1)	5(1)
O(3)	33(2)	38(2)	39(2)	27(2)	12(2)	12(2)
O(4)	35(2)	34(2)	43(2)	26(2)	14(2)	7(2)
N(5)	13(2)	22(2)	24(2)	12(2)	-1(1)	1(1)

N(6)	15(2)	16(2)	16(2)	7(1)	1(1)	3(1)
N(7)	17(2)	15(2)	13(2)	5(1)	3(1)	3(1)
N(8)	21(2)	16(2)	16(2)	7(1)	6(1)	6(1)
C(19)	20(2)	32(3)	37(3)	20(2)	4(2)	-1(2)
C(20)	26(2)	27(2)	36(3)	21(2)	5(2)	2(2)
C(21)	25(2)	22(2)	22(2)	14(2)	4(2)	7(2)
C(22)	14(2)	14(2)	14(2)	3(2)	2(1)	2(1)
C(23)	18(2)	19(2)	18(2)	8(2)	1(2)	7(2)
C(24)	15(2)	20(2)	21(2)	4(2)	1(2)	5(2)
C(25)	16(2)	16(2)	19(2)	4(2)	5(2)	3(2)
C(26)	16(2)	14(2)	14(2)	3(2)	6(2)	3(2)
C(27)	18(2)	22(2)	27(2)	8(2)	7(2)	3(2)
C(28)	23(2)	24(2)	26(2)	8(2)	12(2)	0(2)
C(29)	26(2)	16(2)	17(2)	5(2)	9(2)	8(2)
C(30)	32(2)	19(2)	22(2)	9(2)	13(2)	10(2)
C(31)	40(3)	49(3)	40(3)	34(3)	-23(3)	-13(3)
C(32)	45(3)	33(3)	35(3)	4(2)	-21(2)	20(2)
C(33)	19(2)	64(4)	25(3)	16(2)	-3(2)	12(2)
C(34)	34(3)	30(3)	38(3)	17(2)	-22(2)	-10(2)
C(35)	47(3)	42(3)	27(3)	-9(2)	-20(2)	25(3)
C(36)	20(2)	112(6)	13(2)	21(3)	-1(2)	11(3)
Cl(3)	53(1)	87(1)	72(1)	20(1)	8(1)	23(1)
Cl(4)	50(2)	47(2)	48(2)	13(2)	5(2)	17(2)
Cl(4')	49(1)	41(1)	53(1)	26(1)	8(1)	21(1)
O(5)	22(2)	127(6)	163(7)	-68(5)	2(3)	9(3)
O(6)	105(6)	234(11)	252(13)	191(11)	81(7)	94(7)

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for complex **6** (ic16135). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	6639(1)	6175(1)	6562(1)	19(1)
Cl(1)	3936(2)	5555(1)	6727(1)	23(1)
O(1)	9163(7)	3875(4)	10755(3)	45(1)
O(2)	8792(6)	3641(3)	9228(3)	41(1)
N(1)	5180(6)	7578(3)	6036(3)	23(1)
N(2)	4298(6)	8160(3)	6717(3)	24(1)
N(3)	5609(5)	6900(3)	7842(3)	19(1)
N(4)	6971(6)	5578(3)	8919(3)	23(1)
C(1)	4785(7)	8084(4)	5179(4)	26(1)
C(2)	3639(7)	9022(5)	5310(5)	30(1)
C(3)	3361(7)	9051(4)	6285(4)	28(1)
C(4)	4512(6)	7781(4)	7694(4)	22(1)
C(5)	3582(7)	8353(5)	8435(4)	29(1)
C(6)	3890(8)	7957(5)	9377(5)	32(1)
C(7)	5052(7)	7023(4)	9575(4)	27(1)
C(8)	5886(7)	6487(4)	8801(4)	23(1)
C(9)	5410(8)	6565(5)	10543(4)	30(1)
C(10)	6543(7)	5658(5)	10666(4)	30(1)
C(11)	7304(7)	5184(5)	9836(4)	26(1)
C(12)	8533(7)	4168(5)	9987(4)	28(1)
C(13)	7938(7)	4619(4)	6155(4)	25(1)
C(14)	7906(7)	5376(4)	5326(4)	24(1)
C(15)	8554(6)	6301(4)	5368(4)	23(1)
C(16)	9275(6)	6531(4)	6224(4)	21(1)
C(17)	9258(6)	5757(4)	7035(4)	24(1)
C(18)	8617(7)	4820(4)	7004(4)	22(1)
C(19)	7234(8)	3639(5)	6119(5)	33(1)
C(20)	9954(7)	7520(4)	6263(4)	26(1)
C(21)	9686(10)	7882(5)	7276(5)	46(2)
C(22)	9250(9)	8394(5)	5508(6)	44(2)
Cl(2)	406(2)	10669(1)	7705(1)	42(1)

O(3)	7670(8)	7650(4)	3365(3)	57(2)
C(23)	7410(10)	7043(5)	2628(5)	45(2)
O(4)	10343(10)	1755(4)	9516(4)	75(2)
C(24)	11518(12)	1275(7)	10197(7)	64(2)
O(5)	-3497(8)	11341(6)	8268(7)	91(2)
C(25)	-4227(13)	10569(8)	7878(10)	85(3)

Table S5. Bond lengths [Å] and angles [°] for complex **6** (ic16135).

Ru(1)-N(1)	2.070(4)	C(4)-C(5)	1.420(8)
Ru(1)-N(3)	2.145(4)	C(5)-C(6)	1.368(9)
Ru(1)-C(15)	2.163(5)	C(6)-C(7)	1.403(9)
Ru(1)-C(17)	2.172(5)	C(7)-C(8)	1.405(8)
Ru(1)-C(14)	2.191(5)	C(7)-C(9)	1.430(8)
Ru(1)-C(18)	2.203(5)	C(9)-C(10)	1.354(9)
Ru(1)-C(16)	2.218(5)	C(10)-C(11)	1.412(8)
Ru(1)-C(13)	2.226(6)	C(11)-C(12)	1.501(8)
Ru(1)-Cl(1)	2.4048(12)	C(13)-C(18)	1.400(8)
O(1)-C(12)	1.201(7)	C(13)-C(14)	1.424(8)
O(2)-C(12)	1.310(7)	C(13)-C(19)	1.499(8)
N(1)-C(1)	1.320(7)	C(14)-C(15)	1.410(8)
N(1)-N(2)	1.354(6)	C(15)-C(16)	1.440(7)
N(2)-C(3)	1.363(7)	C(16)-C(17)	1.423(7)
N(2)-C(4)	1.397(7)	C(16)-C(20)	1.500(7)
N(3)-C(4)	1.317(7)	C(17)-C(18)	1.419(8)
N(3)-C(8)	1.392(7)	C(20)-C(22)	1.514(8)
N(4)-C(8)	1.336(7)	C(20)-C(21)	1.520(9)
N(4)-C(11)	1.340(7)	O(3)-C(23)	1.416(9)
C(1)-C(2)	1.409(8)	O(4)-C(24)	1.390(10)
C(2)-C(3)	1.355(9)	O(5)-C(25)	1.429(11)
N(1)-Ru(1)-N(3)	75.47(17)	C(15)-Ru(1)-C(18)	79.8(2)
N(1)-Ru(1)-C(15)	90.93(19)	C(17)-Ru(1)-C(18)	37.9(2)
N(3)-Ru(1)-C(15)	140.89(18)	C(14)-Ru(1)-C(18)	67.1(2)
N(1)-Ru(1)-C(17)	132.65(19)	N(1)-Ru(1)-C(16)	100.23(18)
N(3)-Ru(1)-C(17)	94.86(18)	N(3)-Ru(1)-C(16)	107.35(18)
C(15)-Ru(1)-C(17)	67.58(19)	C(15)-Ru(1)-C(16)	38.36(19)
N(1)-Ru(1)-C(14)	108.8(2)	C(17)-Ru(1)-C(16)	37.82(19)
N(3)-Ru(1)-C(14)	174.72(17)	C(14)-Ru(1)-C(16)	69.2(2)
C(15)-Ru(1)-C(14)	37.8(2)	C(18)-Ru(1)-C(16)	68.83(19)
C(17)-Ru(1)-C(14)	80.0(2)	N(1)-Ru(1)-C(13)	143.6(2)
N(1)-Ru(1)-C(18)	169.02(18)	N(3)-Ru(1)-C(13)	139.08(18)
N(3)-Ru(1)-C(18)	108.11(18)	C(15)-Ru(1)-C(13)	68.1(2)

C(17)-Ru(1)-C(13)	67.7(2)
C(14)-Ru(1)-C(13)	37.6(2)
C(18)-Ru(1)-C(13)	36.9(2)
C(16)-Ru(1)-C(13)	81.78(19)
N(1)-Ru(1)-Cl(1)	84.56(13)
N(3)-Ru(1)-Cl(1)	82.65(11)
C(15)-Ru(1)-Cl(1)	133.19(14)
C(17)-Ru(1)-Cl(1)	141.02(14)
C(14)-Ru(1)-Cl(1)	100.62(14)
C(18)-Ru(1)-Cl(1)	106.07(14)
C(16)-Ru(1)-Cl(1)	169.67(15)
C(13)-Ru(1)-Cl(1)	88.94(14)
C(1)-N(1)-N(2)	106.7(5)
C(1)-N(1)-Ru(1)	137.4(4)
N(2)-N(1)-Ru(1)	115.8(3)
N(1)-N(2)-C(3)	110.5(4)
N(1)-N(2)-C(4)	117.4(4)
C(3)-N(2)-C(4)	132.1(5)
C(4)-N(3)-C(8)	117.8(5)
C(4)-N(3)-Ru(1)	115.9(3)
C(8)-N(3)-Ru(1)	126.1(4)
C(8)-N(4)-C(11)	116.9(5)
N(1)-C(1)-C(2)	109.7(5)
C(3)-C(2)-C(1)	106.3(5)
C(2)-C(3)-N(2)	106.9(5)
N(3)-C(4)-N(2)	115.1(5)
N(3)-C(4)-C(5)	125.4(5)
N(2)-C(4)-C(5)	119.5(5)
C(6)-C(5)-C(4)	116.6(5)
C(5)-C(6)-C(7)	120.3(5)
C(6)-C(7)-C(8)	119.7(5)
C(6)-C(7)-C(9)	122.8(5)
C(8)-C(7)-C(9)	117.4(5)
N(4)-C(8)-N(3)	115.9(5)
N(4)-C(8)-C(7)	124.0(5)
N(3)-C(8)-C(7)	120.1(5)
C(10)-C(9)-C(7)	118.8(5)
C(9)-C(10)-C(11)	119.0(5)
N(4)-C(11)-C(10)	123.8(5)
N(4)-C(11)-C(12)	117.9(5)
C(10)-C(11)-C(12)	118.3(5)
O(1)-C(12)-O(2)	124.5(6)
O(1)-C(12)-C(11)	121.5(6)
O(2)-C(12)-C(11)	114.0(5)
C(18)-C(13)-C(14)	118.5(5)
C(18)-C(13)-C(19)	121.1(5)
C(14)-C(13)-C(19)	120.4(5)
C(18)-C(13)-Ru(1)	70.7(3)
C(14)-C(13)-Ru(1)	69.9(3)
C(19)-C(13)-Ru(1)	130.6(4)
C(15)-C(14)-C(13)	120.2(5)
C(15)-C(14)-Ru(1)	70.1(3)
C(13)-C(14)-Ru(1)	72.5(3)
C(14)-C(15)-C(16)	122.9(5)
C(14)-C(15)-Ru(1)	72.2(3)
C(16)-C(15)-Ru(1)	72.9(3)
C(17)-C(16)-C(15)	114.7(5)
C(17)-C(16)-C(20)	122.7(5)
C(15)-C(16)-C(20)	122.6(5)
C(17)-C(16)-Ru(1)	69.4(3)
C(15)-C(16)-Ru(1)	68.8(3)
C(20)-C(16)-Ru(1)	130.4(4)
C(18)-C(17)-C(16)	123.0(5)
C(18)-C(17)-Ru(1)	72.3(3)
C(16)-C(17)-Ru(1)	72.8(3)
C(13)-C(18)-C(17)	120.6(5)
C(13)-C(18)-Ru(1)	72.5(3)
C(17)-C(18)-Ru(1)	69.9(3)
C(16)-C(20)-C(22)	113.7(5)
C(16)-C(20)-C(21)	112.0(5)
C(22)-C(20)-C(21)	110.5(5)

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($Å^2$ x 10^3) for complex **6** (ic16135). 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)	18(1)	22(1)	15(1)	1(1)	1(1)	-4(1)
Cl(1)	20(1)	29(1)	22(1)	0(1)	1(1)	-9(1)
O(1)	55(3)	46(3)	30(2)	-2(2)	-17(2)	2(2)
O(2)	53(3)	36(2)	27(2)	3(2)	-4(2)	5(2)
N(1)	22(2)	23(2)	23(2)	0(2)	1(2)	-2(2)
N(2)	23(2)	23(2)	24(2)	0(2)	3(2)	-6(2)
N(3)	18(2)	23(2)	16(2)	0(2)	2(2)	-6(2)
N(4)	19(2)	27(2)	23(2)	3(2)	-1(2)	-7(2)
C(1)	22(3)	29(3)	24(3)	9(2)	1(2)	-8(2)
C(2)	23(3)	28(3)	35(3)	8(2)	0(2)	-2(2)
C(3)	23(3)	21(3)	37(3)	1(2)	0(2)	-1(2)
C(4)	18(2)	25(3)	23(3)	-1(2)	5(2)	-9(2)
C(5)	26(3)	27(3)	33(3)	-3(2)	0(2)	-2(2)
C(6)	31(3)	35(3)	29(3)	-12(2)	5(2)	-6(3)
C(7)	30(3)	33(3)	21(3)	-5(2)	1(2)	-12(2)
C(8)	20(2)	28(3)	22(3)	0(2)	3(2)	-10(2)
C(9)	34(3)	39(3)	18(3)	-6(2)	3(2)	-9(3)
C(10)	30(3)	46(3)	14(3)	0(2)	-1(2)	-11(3)
C(11)	22(3)	36(3)	20(3)	1(2)	-5(2)	-8(2)
C(12)	28(3)	35(3)	18(3)	5(2)	0(2)	-7(2)
C(13)	22(3)	26(3)	25(3)	-3(2)	7(2)	-2(2)
C(14)	22(3)	32(3)	18(3)	-5(2)	3(2)	-4(2)
C(15)	16(2)	32(3)	17(3)	4(2)	5(2)	-6(2)
C(16)	9(2)	27(3)	24(3)	3(2)	2(2)	-3(2)
C(17)	19(2)	31(3)	20(3)	0(2)	-3(2)	-2(2)
C(18)	21(3)	25(3)	19(3)	3(2)	1(2)	-2(2)
C(19)	36(3)	24(3)	41(4)	-11(2)	4(3)	-4(3)
C(20)	22(3)	24(3)	32(3)	0(2)	0(2)	-9(2)
C(21)	61(5)	41(4)	43(4)	-6(3)	2(3)	-25(4)
C(22)	46(4)	28(3)	59(5)	12(3)	-20(3)	-13(3)
Cl(2)	36(1)	34(1)	56(1)	-11(1)	10(1)	-5(1)

O(3)	83(4)	64(3)	28(3)	9(2)	-3(3)	-32(3)
C(23)	52(4)	40(4)	44(4)	0(3)	1(3)	-16(3)
O(4)	121(6)	46(3)	42(3)	-5(2)	-21(3)	33(3)
C(24)	71(6)	59(5)	54(5)	3(4)	-16(4)	7(4)
O(5)	54(4)	99(5)	127(7)	-58(5)	11(4)	-8(4)
C(25)	55(5)	61(6)	142(11)	-10(6)	-31(6)	-10(5)