SUPPORTING INFORMATION

Preparation, Reactivity and Structural Peculiarities of Hydroxyalkyl Functionalized "Second Generation" Ruthenium Carbene Complexes

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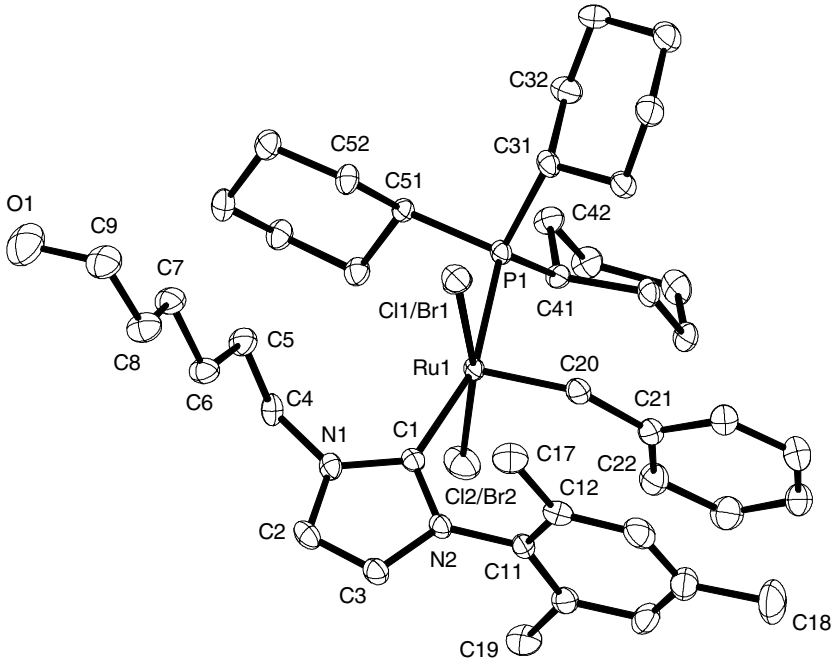

Figure 1. Molecular structure of complex **8a** in the solid state. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are drawn at 50% probability.

Table 1. X-ray structure analysis of complex 8a. Crystal data and structure refinement

Identification code	4322	
Empirical formula	$C_{44}H_{67}Br_{0.50}Cl_{3.50}N_2OPRu$	
Color	red	
Formula weight	936.07 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	**P1, (no. 2)**	
Unit cell dimensions	a = 9.69720(10) Å	α= 80.4820(10)°.
	b = 12.5345(2) Å	β= 85.4340(10)°.
	c = 18.5673(3) Å	γ = 81.6710(10)°.
Volume	2198.72(5) $Å^3$	
Z	2	
Density (calculated)	1.414 $Mg \cdot m^{-3}$	
Absorption coefficient	1.095 mm^{-1}	
F(000)	978 e	

Crystal size	0.13 x 0.09 x 0.03 mm^3	
θ range for data collection	3.49 to 31.17°.	
Index ranges	$-14 \le h \le 13$, $-17 \le k \le 18$, $-27 \le l \le 26$	
Reflections collected	43301	
Independent reflections	13744 [$R_{int} = 0.0751$]	
Reflections with $I>2\sigma(I)$	9880	
Completeness to $\theta = 27.50°$	98.2 %	
Absorption correction	Psi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13744 / 16 / 502	
Goodness-of-fit on F^2	1.075	
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0668$	$wR^2 = 0.1432$
R indices (all data)	$R_1 = 0.1057$	$wR^2 = 0.1588$
Largest diff. peak and hole	1.638 and -1.747 e · $Å^{-3}$	

Table 2. X-ray structure analysis of complex 8a. Atomic coordinates and equivalent isotropic displacement parameters (Å²). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	0.3674(1)	0.0700(1)	0.2003(1)	0.013(1)
Cl(1)	0.1609(6)	0.2048(6)	0.1939(8)	0.020(1)
Cl(2)	0.5833(2)	-0.0448(3)	0.1801(3)	0.012(1)
Br(1)	0.1518(6)	0.2107(5)	0.1931(7)	0.024(1)
Br(2)	0.5882(6)	-0.0565(6)	0.1809(5)	0.035(2)
Cl(3)	0.2280(2)	0.5496(1)	-0.3983(1)	0.056(1)
Cl(4)	0.2946(2)	0.4190(2)	-0.2589(1)	0.095(1)
P(1)	0.4837(1)	0.1772(1)	0.2683(1)	0.015(1)
N(1)	0.3185(3)	0.0508(3)	0.0427(2)	0.017(1)
N(2)	0.2283(3)	-0.0778(3)	0.1129(2)	0.016(1)
O(1)	-0.0409(5)	0.5407(3)	-0.1873(2)	0.050(1)
C(1)	0.2975(4)	0.0092(3)	0.1145(2)	0.015(1)
C(2)	0.2639(4)	-0.0088(4)	-0.0023(2)	0.021(1)
C(3)	0.2065(4)	-0.0880(3)	0.0417(2)	0.020(1)
C(4)	0.3913(4)	0.1458(3)	0.0149(2)	0.020(1)
C(5)	0.2959(5)	0.2543(3)	0.0014(2)	0.023(1)
C(6)	0.1806(5)	0.2568(3)	-0.0504(2)	0.023(1)

C(7)	0.0953(5)	0.3696(4)	-0.0666(3)	0.025(1)
C(8)	-0.0322(5)	0.3686(4)	-0.1079(3)	0.028(1)
C(9)	-0.1162(5)	0.4795(4)	-0.1308(3)	0.033(1)
C(11)	0.1743(4)	-0.1473(3)	0.1748(2)	0.017(1)
C(12)	0.0401(4)	-0.1159(3)	0.2031(2)	0.020(1)
C(13)	-0.0124(5)	-0.1843(4)	0.2632(3)	0.029(1)
C(14)	0.0656(6)	-0.2803(4)	0.2941(3)	0.032(1)
C(15)	0.1973(5)	-0.3112(4)	0.2615(3)	0.029(1)
C(16)	0.2531(5)	-0.2455(3)	0.2016(2)	0.021(1)
C(17)	-0.0453(5)	-0.0124(4)	0.1704(3)	0.027(1)
C(18)	0.0102(7)	-0.3503(5)	0.3606(3)	0.049(2)
C(19)	0.3937(5)	-0.2818(4)	0.1662(3)	0.028(1)
C(20)	0.2809(4)	-0.0118(3)	0.2771(2)	0.020(1)
C(21)	0.3182(5)	-0.1089(3)	0.3315(2)	0.021(1)
C(22)	0.4453(5)	-0.1800(4)	0.3310(3)	0.028(1)
C(23)	0.4701(6)	-0.2682(4)	0.3864(3)	0.034(1)
C(24)	0.3718(6)	-0.2865(4)	0.4443(3)	0.034(1)
C(25)	0.2476(6)	-0.2181(4)	0.4458(3)	0.033(1)
C(26)	0.2201(5)	-0.1299(4)	0.3902(2)	0.027(1)
C(31)	0.3669(4)	0.2640(3)	0.3256(2)	0.018(1)
C(32)	0.4411(5)	0.3308(4)	0.3694(3)	0.025(1)
C(33)	0.3347(5)	0.4113(4)	0.4061(3)	0.030(1)
C(34)	0.2237(5)	0.3544(4)	0.4536(3)	0.030(1)
C(35)	0.1540(5)	0.2861(4)	0.4110(3)	0.027(1)
C(36)	0.2582(5)	0.2047(4)	0.3750(2)	0.022(1)
C(41)	0.6280(4)	0.0978(3)	0.3229(2)	0.017(1)
C(42)	0.7467(4)	0.1557(3)	0.3417(2)	0.022(1)
C(43)	0.8653(5)	0.0698(4)	0.3725(3)	0.026(1)
C(44)	0.8153(5)	-0.0095(4)	0.4384(2)	0.029(1)
C(45)	0.6916(5)	-0.0597(4)	0.4213(2)	0.023(1)
C(46)	0.5746(4)	0.0283(3)	0.3924(2)	0.020(1)
C(51)	0.5747(4)	0.2781(3)	0.2031(2)	0.015(1)
C(52)	0.4732(4)	0.3601(3)	0.1551(2)	0.019(1)
C(53)	0.5515(5)	0.4416(4)	0.1029(2)	0.024(1)
C(54)	0.6675(5)	0.3865(4)	0.0563(2)	0.024(1)
C(55)	0.7677(4)	0.3056(4)	0.1050(2)	0.023(1)
C(56)	0.6899(4)	0.2224(3)	0.1548(2)	0.021(1)
C(99)	0.1898(8)	0.5318(6)	-0.3031(4)	0.057(2)

Table 3. X-ray structure analysis of complex 8a. Bond lengths [Å] and angles [°].

Ru(1)-C(20)	1.834(4)	Ru(1)-C(1)	2.074(4)
Ru(1)-Cl(2)	2.4033(15)	Ru(1)-Cl(1)	2.4230(18)
Ru(1)-P(1)	2.4289(11)	Ru(1)-Br(2)	2.5121(19)
Ru(1)-Br(1)	2.5294(17)	Cl(3)-C(99)	1.761(7)
Cl(4)-C(99)	1.743(8)	P(1)-C(31)	1.853(4)
P(1)-C(41)	1.861(4)	P(1)-C(51)	1.868(4)
N(1)-C(1)	1.359(5)	N(1)-C(2)	1.388(5)
N(1)-C(4)	1.472(5)	N(2)-C(1)	1.366(5)
N(2)-C(3)	1.385(5)	N(2)-C(11)	1.434(5)
O(1)-C(9)	1.413(6)	C(2)-C(3)	1.335(6)
C(4)-C(5)	1.526(6)	C(5)-C(6)	1.526(6)
C(6)-C(7)	1.528(6)	C(7)-C(8)	1.508(6)
C(8)-C(9)	1.519(6)	C(11)-C(16)	1.390(6)
C(11)-C(12)	1.392(6)	C(12)-C(13)	1.399(6)
C(12)-C(17)	1.499(6)	C(13)-C(14)	1.388(7)
C(14)-C(15)	1.399(7)	C(14)-C(18)	1.503(7)
C(15)-C(16)	1.392(6)	C(16)-C(19)	1.508(6)
C(20)-C(21)	1.469(6)	C(21)-C(26)	1.405(6)
C(21)-C(22)	1.412(6)	C(22)-C(23)	1.386(6)
C(23)-C(24)	1.391(7)	C(24)-C(25)	1.375(7)
C(25)-C(26)	1.393(6)	C(31)-C(36)	1.534(6)
C(31)-C(32)	1.541(6)	C(32)-C(33)	1.536(6)
C(33)-C(34)	1.520(7)	C(34)-C(35)	1.514(7)
C(35)-C(36)	1.526(6)	C(41)-C(46)	1.532(5)
C(41)-C(42)	1.538(6)	C(42)-C(43)	1.533(6)
C(43)-C(44)	1.538(6)	C(44)-C(45)	1.510(7)
C(45)-C(46)	1.526(5)	C(51)-C(56)	1.536(5)
C(51)-C(52)	1.537(5)	C(52)-C(53)	1.530(6)
C(53)-C(54)	1.519(6)	C(54)-C(55)	1.529(6)
C(55)-C(56)	1.521(6)		
C(20)-Ru(1)-C(1)	99.21(17)	C(20)-Ru(1)-Cl(2)	102.65(17)
C(1)-Ru(1)-Cl(2)	85.79(16)	C(20)-Ru(1)-Cl(1)	89.1(3)
C(1)-Ru(1)-Cl(1)	88.4(3)	Cl(2)-Ru(1)-Cl(1)	167.6(3)
C(20)-Ru(1)-P(1)	99.12(13)	C(1)-Ru(1)-P(1)	161.66(11)
Cl(2)-Ru(1)-P(1)	90.80(12)	Cl(1)-Ru(1)-P(1)	91.3(3)
C(20)-Ru(1)-Br(2)	100.7(3)	C(1)-Ru(1)-Br(2)	84.9(3)

Cl(1)-Ru(1)-Br(2)	168.9(4)	P(1)-Ru(1)-Br(2)	92.3(2)
C(20)-Ru(1)-Br(1)	89.2(3)	C(1)-Ru(1)-Br(1)	88.2(3)
Cl(2)-Ru(1)-Br(1)	167.4(3)	P(1)-Ru(1)-Br(1)	91.5(2)
Br(2)-Ru(1)-Br(1)	168.7(3)	C(31)-P(1)-C(41)	109.87(18)
C(31)-P(1)-C(51)	103.24(18)	C(41)-P(1)-C(51)	102.86(18)
C(31)-P(1)-Ru(1)	115.42(14)	C(41)-P(1)-Ru(1)	114.56(14)
C(51)-P(1)-Ru(1)	109.52(13)	C(1)-N(1)-C(2)	111.5(3)
C(1)-N(1)-C(4)	125.1(4)	C(2)-N(1)-C(4)	123.4(3)
C(1)-N(2)-C(3)	110.9(3)	C(1)-N(2)-C(11)	126.7(3)
C(3)-N(2)-C(11)	122.2(3)	N(1)-C(1)-N(2)	103.7(3)
N(1)-C(1)-Ru(1)	124.4(3)	N(2)-C(1)-Ru(1)	131.9(3)
C(3)-C(2)-N(1)	106.6(4)	C(2)-C(3)-N(2)	107.3(4)
N(1)-C(4)-C(5)	114.6(3)	C(6)-C(5)-C(4)	114.6(4)
C(5)-C(6)-C(7)	112.4(4)	C(8)-C(7)-C(6)	112.6(4)
C(7)-C(8)-C(9)	115.5(4)	O(1)-C(9)-C(8)	109.7(4)
C(16)-C(11)-C(12)	122.3(4)	C(16)-C(11)-N(2)	119.6(4)
C(12)-C(11)-N(2)	118.0(4)	C(11)-C(12)-C(13)	117.7(4)
C(11)-C(12)-C(17)	121.1(4)	C(13)-C(12)-C(17)	121.2(4)
C(14)-C(13)-C(12)	121.7(4)	C(13)-C(14)-C(15)	118.5(4)
C(13)-C(14)-C(18)	121.1(5)	C(15)-C(14)-C(18)	120.5(5)
C(16)-C(15)-C(14)	121.5(4)	C(11)-C(16)-C(15)	118.1(4)
C(11)-C(16)-C(19)	121.4(4)	C(15)-C(16)-C(19)	120.5(4)
C(21)-C(20)-Ru(1)	137.8(3)	C(26)-C(21)-C(22)	117.8(4)
C(26)-C(21)-C(20)	116.5(4)	C(22)-C(21)-C(20)	125.7(4)
C(23)-C(22)-C(21)	120.5(5)	C(22)-C(23)-C(24)	120.6(5)
C(25)-C(24)-C(23)	119.7(4)	C(24)-C(25)-C(26)	120.5(5)
C(25)-C(26)-C(21)	120.9(5)	C(36)-C(31)-C(32)	110.5(3)
C(36)-C(31)-P(1)	114.5(3)	C(32)-C(31)-P(1)	115.3(3)
C(33)-C(32)-C(31)	110.8(4)	C(34)-C(33)-C(32)	112.1(4)
C(35)-C(34)-C(33)	111.2(4)	C(34)-C(35)-C(36)	112.8(4)
C(35)-C(36)-C(31)	110.4(4)	C(46)-C(41)-C(42)	109.0(3)
C(46)-C(41)-P(1)	112.5(3)	C(42)-C(41)-P(1)	119.7(3)
C(43)-C(42)-C(41)	109.2(3)	C(42)-C(43)-C(44)	112.5(4)
C(45)-C(44)-C(43)	111.6(4)	C(44)-C(45)-C(46)	111.0(4)
C(45)-C(46)-C(41)	109.7(3)	C(56)-C(51)-C(52)	110.1(3)
C(56)-C(51)-P(1)	112.2(3)	C(52)-C(51)-P(1)	112.6(3)
C(53)-C(52)-C(51)	110.9(3)	C(54)-C(53)-C(52)	112.8(4)
C(53)-C(54)-C(55)	110.3(4)	C(56)-C(55)-C(54)	110.9(4)
C(55)-C(56)-C(51)	111.4(3)	Cl(4)-C(99)-Cl(3)	111.1(4)

Table 4. X-ray structure analysis of complex 8a. Anisotropic displacement parameters (Å^2). 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)	0.014(1)	0.014(1)	0.011(1)	-0.001(1)	-0.002(1)	0.001(1)
Cl(1)	0.020(2)	0.014(2)	0.025(3)	-0.002(2)	-0.004(2)	-0.001(1)
Cl(2)	0.008(1)	0.015(1)	0.012(1)	-0.004(1)	0.001(1)	-0.002(1)
Br(1)	0.026(2)	0.022(2)	0.021(2)	-0.003(1)	-0.006(1)	0.008(1)
Br(2)	0.036(3)	0.035(3)	0.031(3)	-0.010(2)	-0.007(2)	0.009(2)
Cl(3)	0.059(1)	0.056(1)	0.058(1)	-0.007(1)	0.009(1)	-0.026(1)
Cl(4)	0.069(1)	0.154(2)	0.049(1)	-0.021(1)	-0.018(1)	0.040(1)
P(1)	0.017(1)	0.016(1)	0.012(1)	-0.001(1)	-0.003(1)	0.001(1)
N(1)	0.016(2)	0.019(2)	0.014(2)	0.000(1)	-0.003(1)	0.002(1)
N(2)	0.019(2)	0.018(2)	0.012(2)	-0.003(1)	-0.003(1)	-0.001(1)
O(1)	0.053(3)	0.034(2)	0.051(3)	0.007(2)	0.004(2)	0.010(2)
C(1)	0.014(2)	0.015(2)	0.014(2)	-0.003(1)	-0.001(1)	0.003(1)
C(2)	0.021(2)	0.027(2)	0.015(2)	-0.006(2)	-0.005(2)	0.001(2)
C(3)	0.023(2)	0.022(2)	0.016(2)	-0.004(2)	-0.004(2)	-0.002(2)
C(4)	0.020(2)	0.026(2)	0.014(2)	0.002(2)	-0.002(2)	-0.004(2)
C(5)	0.026(2)	0.020(2)	0.022(2)	-0.001(2)	-0.006(2)	-0.002(2)
C(6)	0.028(2)	0.018(2)	0.024(2)	-0.004(2)	-0.008(2)	0.001(2)
C(7)	0.032(2)	0.019(2)	0.025(2)	-0.004(2)	-0.007(2)	0.001(2)
C(8)	0.027(2)	0.023(2)	0.034(2)	-0.004(2)	-0.010(2)	0.001(2)
C(9)	0.033(3)	0.027(2)	0.036(3)	-0.003(2)	-0.008(2)	0.004(2)
C(11)	0.018(2)	0.018(2)	0.014(2)	-0.003(1)	0.000(1)	-0.002(2)
C(12)	0.018(2)	0.021(2)	0.023(2)	-0.009(2)	-0.002(2)	-0.001(2)
C(13)	0.028(2)	0.034(3)	0.028(2)	-0.012(2)	0.009(2)	-0.010(2)
C(14)	0.045(3)	0.031(3)	0.022(2)	-0.002(2)	-0.002(2)	-0.016(2)
C(15)	0.040(3)	0.021(2)	0.024(2)	0.003(2)	-0.010(2)	-0.006(2)
C(16)	0.025(2)	0.020(2)	0.018(2)	-0.003(2)	-0.006(2)	-0.001(2)
C(17)	0.020(2)	0.027(2)	0.035(3)	-0.008(2)	-0.002(2)	0.003(2)
C(18)	0.067(4)	0.056(4)	0.027(3)	0.002(3)	0.006(3)	-0.036(3)
C(19)	0.022(2)	0.026(2)	0.034(2)	-0.006(2)	-0.008(2)	0.005(2)
C(20)	0.023(2)	0.020(2)	0.016(2)	-0.004(2)	-0.004(2)	-0.002(2)
C(21)	0.026(2)	0.020(2)	0.017(2)	-0.003(2)	-0.003(2)	-0.002(2)
C(22)	0.031(2)	0.027(2)	0.023(2)	-0.001(2)	-0.005(2)	0.001(2)

C(23)	0.043(3)	0.029(2)	0.028(2)	-0.002(2)	-0.012(2)	0.002(2)
C(24)	0.057(3)	0.026(2)	0.018(2)	0.002(2)	-0.010(2)	-0.002(2)
C(25)	0.045(3)	0.034(3)	0.021(2)	-0.003(2)	0.002(2)	-0.008(2)
C(26)	0.034(2)	0.025(2)	0.022(2)	-0.002(2)	0.001(2)	-0.003(2)
C(31)	0.019(2)	0.020(2)	0.013(2)	-0.002(1)	-0.002(1)	0.004(2)
C(32)	0.027(2)	0.024(2)	0.025(2)	-0.009(2)	-0.002(2)	0.000(2)
C(33)	0.043(3)	0.018(2)	0.028(2)	-0.009(2)	0.004(2)	0.001(2)
C(34)	0.038(3)	0.026(2)	0.021(2)	-0.004(2)	0.002(2)	0.006(2)
C(35)	0.028(2)	0.025(2)	0.025(2)	-0.003(2)	0.007(2)	0.005(2)
C(36)	0.024(2)	0.022(2)	0.018(2)	-0.005(2)	0.002(2)	0.000(2)
C(41)	0.019(2)	0.014(2)	0.016(2)	-0.002(1)	-0.005(1)	0.002(1)
C(42)	0.024(2)	0.019(2)	0.025(2)	-0.002(2)	-0.009(2)	-0.002(2)
C(43)	0.024(2)	0.027(2)	0.026(2)	-0.002(2)	-0.011(2)	-0.002(2)
C(44)	0.028(2)	0.033(2)	0.021(2)	-0.001(2)	-0.010(2)	0.009(2)
C(45)	0.030(2)	0.020(2)	0.017(2)	0.002(2)	-0.006(2)	0.004(2)
C(46)	0.022(2)	0.021(2)	0.013(2)	0.001(2)	-0.004(2)	0.003(2)
C(51)	0.016(2)	0.014(2)	0.014(2)	-0.001(1)	-0.001(1)	0.000(1)
C(52)	0.018(2)	0.021(2)	0.017(2)	0.003(2)	-0.003(2)	0.001(2)
C(53)	0.028(2)	0.021(2)	0.020(2)	0.002(2)	-0.004(2)	0.002(2)
C(54)	0.027(2)	0.026(2)	0.017(2)	0.002(2)	-0.002(2)	-0.005(2)
C(55)	0.021(2)	0.023(2)	0.023(2)	-0.001(2)	0.001(2)	-0.004(2)
C(56)	0.020(2)	0.020(2)	0.020(2)	0.000(2)	-0.001(2)	0.001(2)
C(99)	0.058(4)	0.058(4)	0.061(4)	-0.022(3)	-0.007(3)	-0.017(3)

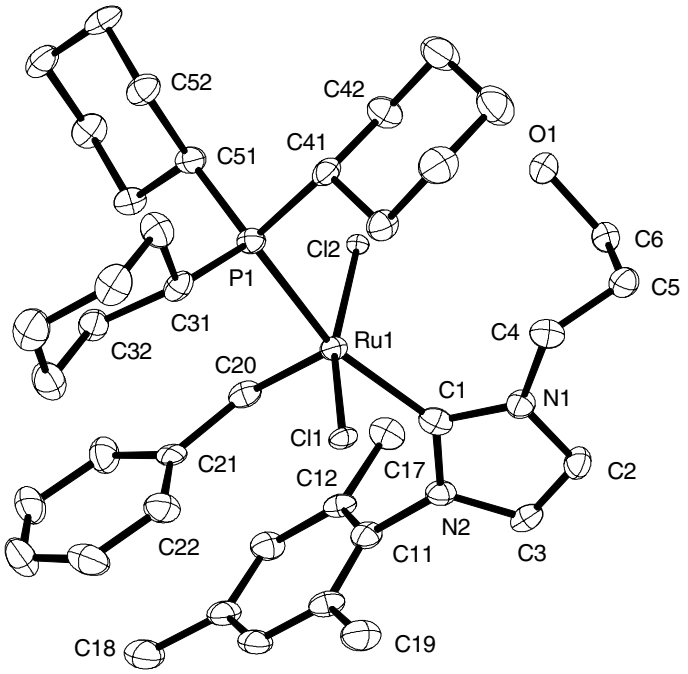

Figure 2. Molecular structure of complex **8b** in the solid state. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are drawn at 50% probability.

Table 5. X-ray structure analysis of complex 8b. Crystal data and structure refinement.

Empirical formula	$C_{41.50}H_{62}Cl_5N_2OPRu$	
Color	red	
Formula weight	914.22 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	**$P2_1/n$, (no. 14)**	
Unit cell dimensions	a = 17.3808(9) Å	α= 90°.
	b = 12.0539(7) Å	β= 106.951(2)°.
	c = 22.7446(12) Å	γ = 90°.
Volume	4558.1(4) $Å^3$	
Z	4	
Density (calculated)	1.332 $Mg \cdot m^{-3}$	
Absorption coefficient	0.704 mm^{-1}	
F(000)	1908 e	
Crystal size	0.22 x 0.19 x 0.12 mm^3	

θ range for data collection	1.74 to 23.27°.	
Index ranges	$-19 \le h \le 19$, $-13 \le k \le 6$, $-23 \le l \le 25$	
Reflections collected	30188	
Independent reflections	6527 [$R_{int} = 0.1047$]	
Reflections with $I>2\sigma(I)$	4498	
Completeness to $\theta = 23.27°$	99.5 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.9202 and 0.8604	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6527 / 0 / 482	
Goodness-of-fit on F^2	1.056	
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0508$	$wR^2 = 0.1252$
R indices (all data)	$R_1 = 0.0890$	$wR^2 = 0.1413$
Largest diff. peak and hole	1.229 and -0.708 e · Å^{-3}	

Table 6. X-ray structure analysis of complex 8b. Atomic coordinates and equivalent isotropic displacement parameters (Å^2). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	1.1760(1)	1.0731(1)	0.4214(1)	0.017(1)
P(1)	1.2871(1)	1.1941(1)	0.4697(1)	0.018(1)
O(1)	1.2603(2)	0.7948(4)	0.5494(2)	0.026(1)
N(1)	1.0646(3)	0.9101(4)	0.4556(2)	0.020(1)
C(1)	1.0833(4)	0.9614(5)	0.4083(3)	0.020(2)
Cl(1)	1.0822(1)	1.2103(1)	0.4362(1)	0.016(1)
N(2)	1.0275(3)	0.9201(4)	0.3574(2)	0.019(1)
C(2)	0.9991(4)	0.8399(5)	0.4355(3)	0.023(2)
Cl(2)	1.2683(1)	0.9186(1)	0.4305(1)	0.012(1)
C(3)	0.9767(4)	0.8463(5)	0.3738(3)	0.024(2)
C(4)	1.1074(4)	0.9323(5)	0.5202(3)	0.023(2)
C(5)	1.1267(4)	0.8287(5)	0.5584(3)	0.023(2)
C(6)	1.1813(3)	0.7496(5)	0.5376(3)	0.024(2)
C(11)	1.0238(3)	0.9467(5)	0.2944(3)	0.021(2)
C(12)	1.0678(3)	0.8820(5)	0.2654(3)	0.020(2)
C(13)	1.0644(3)	0.9113(5)	0.2056(3)	0.023(2)

C(14)	1.0189(4)	1.0006(5)	0.1761(3)	0.023(2)
C(15)	0.9743(4)	1.0593(6)	0.2064(3)	0.024(2)
C(16)	0.9754(4)	1.0347(5)	0.2662(3)	0.023(2)
C(17)	1.1165(4)	0.7845(5)	0.2966(3)	0.028(2)
C(18)	1.0180(4)	1.0316(7)	0.1119(3)	0.036(2)
C(19)	0.9266(4)	1.0990(6)	0.2992(3)	0.032(2)
C(20)	1.1771(3)	1.0892(5)	0.3419(3)	0.019(1)
C(21)	1.1512(3)	1.1742(5)	0.2936(3)	0.019(1)
C(22)	1.1016(4)	1.2632(6)	0.2949(3)	0.028(2)
C(23)	1.0838(4)	1.3408(6)	0.2482(3)	0.036(2)
C(24)	1.1173(4)	1.3322(6)	0.1996(3)	0.039(2)
C(25)	1.1662(4)	1.2437(6)	0.1971(3)	0.033(2)
C(26)	1.1826(4)	1.1654(6)	0.2433(3)	0.028(2)
C(31)	1.2654(4)	1.3443(5)	0.4562(3)	0.021(2)
C(32)	1.2678(4)	1.3845(5)	0.3931(3)	0.024(2)
C(33)	1.2288(4)	1.4978(6)	0.3786(3)	0.034(2)
C(34)	1.2687(4)	1.5828(6)	0.4280(3)	0.037(2)
C(35)	1.2727(4)	1.5408(5)	0.4915(3)	0.032(2)
C(36)	1.3110(4)	1.4270(5)	0.5044(3)	0.028(2)
C(41)	1.3101(3)	1.1836(5)	0.5543(3)	0.021(2)
C(42)	1.3454(4)	1.0705(6)	0.5803(3)	0.026(2)
C(43)	1.3680(4)	1.0720(7)	0.6502(3)	0.036(2)
C(44)	1.2968(4)	1.1022(6)	0.6733(3)	0.038(2)
C(45)	1.2611(4)	1.2128(6)	0.6472(3)	0.035(2)
C(46)	1.2377(4)	1.2122(6)	0.5765(3)	0.024(2)
C(51)	1.3847(3)	1.1591(5)	0.4562(3)	0.021(1)
C(52)	1.4548(3)	1.2336(5)	0.4908(3)	0.025(2)
C(53)	1.5348(4)	1.1919(6)	0.4827(3)	0.029(2)
C(54)	1.5300(4)	1.1829(6)	0.4150(3)	0.027(2)
C(55)	1.4608(4)	1.1081(5)	0.3809(3)	0.025(2)
C(56)	1.3801(3)	1.1479(5)	0.3882(3)	0.022(2)
Cl(60)	0.7761(1)	0.9334(2)	0.1763(1)	0.077(1)
C(60)	0.8438(4)	0.8275(7)	0.1751(3)	0.046(2)
Cl(61)	0.8362(2)	0.7169(2)	0.2237(1)	0.094(1)
Cl(70)	0.9153(2)	0.5519(3)	0.4380(2)	0.045(1)
C(70)	0.9699(13)	0.4910(17)	0.3998(9)	0.084(7)
Cl(71)	0.9639(3)	0.5178(4)	0.3287(2)	0.069(1)

Table 7. X-ray structure analysis of complex 8b. Bond lengths [Å] and angles [°].

Ru(1)-C(20)	1.825(6)	Ru(1)-C(1)	2.052(6)
Ru(1)-Cl(1)	2.4134(15)	Ru(1)-P(1)	2.4142(16)
Ru(1)-Cl(2)	2.4273(14)	P(1)-C(41)	1.851(6)
P(1)-C(31)	1.857(6)	P(1)-C(51)	1.860(6)
O(1)-C(6)	1.428(7)	N(1)-C(1)	1.362(8)
N(1)-C(2)	1.384(8)	N(1)-C(4)	1.465(7)
C(1)-N(2)	1.369(7)	N(2)-C(3)	1.380(8)
N(2)-C(11)	1.451(7)	C(2)-C(3)	1.345(8)
C(4)-C(5)	1.502(9)	C(5)-C(6)	1.515(8)
C(11)-C(12)	1.385(8)	C(11)-C(16)	1.389(9)
C(12)-C(13)	1.390(8)	C(12)-C(17)	1.501(9)
C(13)-C(14)	1.388(9)	C(14)-C(15)	1.374(9)
C(14)-C(18)	1.503(9)	C(15)-C(16)	1.388(9)
C(16)-C(19)	1.500(9)	C(20)-C(21)	1.472(8)
C(21)-C(22)	1.382(9)	C(21)-C(26)	1.408(9)
C(22)-C(23)	1.382(9)	C(23)-C(24)	1.394(10)
C(24)-C(25)	1.375(10)	C(25)-C(26)	1.380(9)
C(31)-C(36)	1.522(9)	C(31)-C(32)	1.527(8)
C(32)-C(33)	1.518(9)	C(33)-C(34)	1.530(10)
C(34)-C(35)	1.513(9)	C(35)-C(36)	1.516(9)
C(41)-C(46)	1.524(8)	C(41)-C(42)	1.540(9)
C(42)-C(43)	1.522(9)	C(43)-C(44)	1.525(10)
C(44)-C(45)	1.517(10)	C(45)-C(46)	1.540(8)
C(51)-C(56)	1.531(8)	C(51)-C(52)	1.533(8)
C(52)-C(53)	1.540(8)	C(53)-C(54)	1.520(9)
C(54)-C(55)	1.523(9)	C(55)-C(56)	1.537(8)
Cl(60)-C(60)	1.743(8)	C(60)-Cl(61)	1.761(8)
Cl(70)-C(70)	1.635(16)	C(70)-Cl(71)	1.623(18)
C(20)-Ru(1)-C(1)	99.2(2)	C(20)-Ru(1)-Cl(1)	105.5(2)
C(1)-Ru(1)-Cl(1)	86.39(16)	C(20)-Ru(1)-P(1)	98.52(18)
C(1)-Ru(1)-P(1)	162.18(17)	Cl(1)-Ru(1)-P(1)	90.29(5)
C(20)-Ru(1)-Cl(2)	88.2(2)	C(1)-Ru(1)-Cl(2)	88.90(16)
Cl(1)-Ru(1)-Cl(2)	166.07(5)	P(1)-Ru(1)-Cl(2)	90.20(5)
C(41)-P(1)-C(31)	102.2(3)	C(41)-P(1)-C(51)	103.0(3)
C(31)-P(1)-C(51)	110.2(3)	C(41)-P(1)-Ru(1)	109.5(2)

C(31)-P(1)-Ru(1)	114.7(2)	C(51)-P(1)-Ru(1)	115.8(2)
C(1)-N(1)-C(2)	112.3(5)	C(1)-N(1)-C(4)	122.8(5)
C(2)-N(1)-C(4)	124.8(5)	N(1)-C(1)-N(2)	103.3(5)
N(1)-C(1)-Ru(1)	122.8(4)	N(2)-C(1)-Ru(1)	133.9(4)
C(1)-N(2)-C(3)	110.9(5)	C(1)-N(2)-C(11)	124.9(5)
C(3)-N(2)-C(11)	124.2(5)	C(3)-C(2)-N(1)	105.7(5)
C(2)-C(3)-N(2)	107.8(5)	N(1)-C(4)-C(5)	113.0(5)
C(4)-C(5)-C(6)	113.4(5)	O(1)-C(6)-C(5)	110.9(5)
C(12)-C(11)-C(16)	123.7(6)	C(12)-C(11)-N(2)	118.3(5)
C(16)-C(11)-N(2)	118.0(5)	C(11)-C(12)-C(13)	116.8(6)
C(11)-C(12)-C(17)	121.9(6)	C(13)-C(12)-C(17)	121.2(6)
C(14)-C(13)-C(12)	121.6(6)	C(15)-C(14)-C(13)	118.9(6)
C(15)-C(14)-C(18)	120.7(6)	C(13)-C(14)-C(18)	120.3(6)
C(14)-C(15)-C(16)	122.1(6)	C(15)-C(16)-C(11)	116.7(6)
C(15)-C(16)-C(19)	122.0(6)	C(11)-C(16)-C(19)	121.3(6)
C(21)-C(20)-Ru(1)	136.3(5)	C(22)-C(21)-C(26)	117.9(6)
C(22)-C(21)-C(20)	125.6(6)	C(26)-C(21)-C(20)	116.5(6)
C(23)-C(22)-C(21)	120.7(6)	C(22)-C(23)-C(24)	120.5(7)
C(25)-C(24)-C(23)	119.8(7)	C(24)-C(25)-C(26)	119.4(6)
C(25)-C(26)-C(21)	121.7(7)	C(36)-C(31)-C(32)	108.5(5)
C(36)-C(31)-P(1)	118.8(4)	C(32)-C(31)-P(1)	113.9(4)
C(33)-C(32)-C(31)	110.9(5)	C(32)-C(33)-C(34)	111.4(5)
C(35)-C(34)-C(33)	111.2(6)	C(34)-C(35)-C(36)	112.5(6)
C(35)-C(36)-C(31)	110.3(5)	C(46)-C(41)-C(42)	110.4(5)
C(46)-C(41)-P(1)	112.3(4)	C(42)-C(41)-P(1)	113.6(4)
C(43)-C(42)-C(41)	110.1(6)	C(42)-C(43)-C(44)	112.0(6)
C(45)-C(44)-C(43)	110.8(6)	C(44)-C(45)-C(46)	111.0(6)
C(41)-C(46)-C(45)	110.8(5)	C(56)-C(51)-C(52)	111.7(5)
C(56)-C(51)-P(1)	114.0(4)	C(52)-C(51)-P(1)	114.2(4)
C(51)-C(52)-C(53)	111.0(5)	C(54)-C(53)-C(52)	111.1(5)
C(53)-C(54)-C(55)	111.1(5)	C(54)-C(55)-C(56)	111.7(5)
C(51)-C(56)-C(55)	110.9(5)	Cl(60)-C(60)-Cl(61)	111.7(4)
Cl(71)-C(70)-Cl(70)	124.1(10)		

Table 8. X-ray structure analysis of complex 8b. Anisotropic displacement parameters (Å^2). 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)	0.014(1)	0.019(1)	0.017(1)	-0.001(1)	0.004(1)	0.000(1)
P(1)	0.016(1)	0.017(1)	0.020(1)	0.000(1)	0.004(1)	0.001(1)
O(1)	0.021(2)	0.029(3)	0.028(3)	0.005(2)	0.009(2)	-0.001(2)
N(1)	0.020(3)	0.022(3)	0.017(3)	-0.003(2)	0.005(2)	-0.003(2)
C(1)	0.021(3)	0.019(4)	0.020(3)	-0.002(3)	0.006(3)	0.009(3)
Cl(1)	0.010(1)	0.023(1)	0.015(1)	-0.003(1)	0.004(1)	0.002(1)
N(2)	0.017(3)	0.025(3)	0.015(3)	-0.002(2)	0.002(2)	0.000(3)
C(2)	0.024(4)	0.021(4)	0.025(4)	0.000(3)	0.008(3)	-0.006(3)
Cl(2)	0.010(1)	0.013(1)	0.012(1)	0.001(1)	0.002(1)	0.001(1)
C(3)	0.015(3)	0.027(4)	0.029(4)	-0.002(3)	0.005(3)	-0.003(3)
C(4)	0.023(3)	0.024(4)	0.020(3)	-0.004(3)	0.004(3)	0.003(3)
C(5)	0.020(3)	0.029(4)	0.023(4)	0.001(3)	0.008(3)	0.000(3)
C(6)	0.022(4)	0.023(4)	0.026(4)	0.006(3)	0.007(3)	0.000(3)
C(11)	0.019(3)	0.028(4)	0.015(3)	-0.005(3)	0.002(3)	-0.005(3)
C(12)	0.014(3)	0.021(4)	0.022(4)	-0.004(3)	0.000(3)	-0.001(3)
C(13)	0.021(3)	0.030(4)	0.017(3)	-0.005(3)	0.004(3)	0.001(3)
C(14)	0.016(3)	0.031(4)	0.020(3)	-0.002(3)	0.000(3)	-0.001(3)
C(15)	0.019(3)	0.029(4)	0.020(3)	0.000(3)	-0.003(3)	0.000(3)
C(16)	0.017(3)	0.025(4)	0.022(4)	-0.008(3)	0.000(3)	-0.002(3)
C(17)	0.029(4)	0.027(4)	0.026(4)	0.001(3)	0.005(3)	0.003(3)
C(18)	0.026(4)	0.054(5)	0.025(4)	0.004(4)	0.000(3)	0.001(4)
C(19)	0.024(4)	0.040(5)	0.031(4)	-0.001(3)	0.005(3)	0.005(3)
C(20)	0.017(3)	0.017(3)	0.022(3)	-0.008(3)	0.002(3)	-0.004(3)
C(21)	0.014(3)	0.017(3)	0.020(3)	-0.002(3)	-0.005(3)	-0.006(3)
C(22)	0.024(4)	0.030(4)	0.028(4)	0.002(3)	0.005(3)	0.006(3)
C(23)	0.035(4)	0.032(4)	0.033(4)	0.004(4)	-0.003(3)	0.005(4)
C(24)	0.046(5)	0.039(5)	0.031(4)	0.016(4)	0.006(4)	-0.001(4)
C(25)	0.037(4)	0.042(5)	0.023(4)	0.009(3)	0.013(3)	0.002(4)
C(26)	0.033(4)	0.032(4)	0.022(4)	0.001(3)	0.011(3)	-0.004(3)
C(31)	0.016(3)	0.019(4)	0.031(4)	-0.002(3)	0.011(3)	0.001(3)
C(32)	0.023(4)	0.022(4)	0.027(4)	0.001(3)	0.009(3)	0.000(3)
C(33)	0.039(4)	0.030(4)	0.033(4)	0.008(3)	0.011(3)	0.003(4)

C(34)	0.038(4)	0.025(4)	0.051(5)	0.002(4)	0.019(4)	0.003(4)
C(35)	0.035(4)	0.022(4)	0.044(4)	-0.007(3)	0.018(3)	0.000(3)
C(36)	0.035(4)	0.024(4)	0.023(3)	-0.001(3)	0.007(3)	-0.001(3)
C(41)	0.016(3)	0.024(4)	0.023(3)	-0.002(3)	0.005(3)	-0.006(3)
C(42)	0.029(4)	0.028(4)	0.021(3)	0.000(3)	0.005(3)	0.004(3)
C(43)	0.036(4)	0.041(4)	0.027(4)	0.008(4)	0.005(3)	0.008(4)
C(44)	0.045(5)	0.045(5)	0.025(4)	0.006(3)	0.010(3)	0.003(4)
C(45)	0.033(4)	0.048(5)	0.024(4)	-0.009(4)	0.010(3)	-0.003(4)
C(46)	0.022(3)	0.030(4)	0.021(3)	-0.003(3)	0.008(3)	-0.001(3)
C(51)	0.018(3)	0.013(3)	0.028(4)	0.001(3)	0.002(3)	0.000(3)
C(52)	0.021(3)	0.021(4)	0.034(4)	-0.003(3)	0.007(3)	-0.002(3)
C(53)	0.014(3)	0.032(4)	0.038(4)	-0.006(3)	0.003(3)	-0.007(3)
C(54)	0.017(3)	0.025(4)	0.042(4)	0.000(3)	0.012(3)	0.000(3)
C(55)	0.025(4)	0.023(4)	0.032(4)	-0.005(3)	0.013(3)	0.004(3)
C(56)	0.018(3)	0.023(4)	0.022(3)	-0.003(3)	0.004(3)	0.000(3)
Cl(60)	0.040(1)	0.107(2)	0.082(2)	-0.056(2)	0.012(1)	0.001(1)
C(60)	0.035(4)	0.066(6)	0.040(5)	-0.014(4)	0.017(4)	-0.012(4)
Cl(61)	0.167(3)	0.078(2)	0.047(1)	-0.019(1)	0.044(2)	-0.044(2)
Cl(70)	0.044(2)	0.037(2)	0.062(3)	-0.004(2)	0.027(2)	-0.001(2)
C(70)	0.122(18)	0.068(14)	0.076(14)	0.026(11)	0.047(13)	0.083(14)
Cl(71)	0.088(4)	0.063(3)	0.063(3)	0.005(3)	0.033(3)	0.013(3)

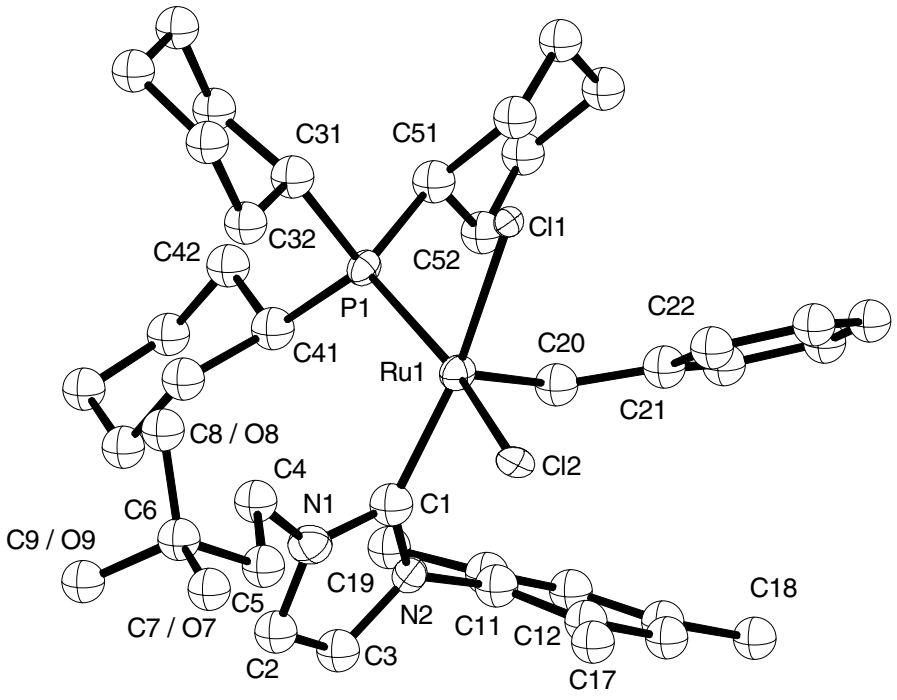

Figure 3. Molecular structure of complex **10** in the solid state. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are drawn at 50% probability.

Table 9. X-ray structure analysis of complex 10. Crystal data and structure refinement.

Empirical formula	$C_{42.75}H_{57.50}Cl_2N_2O_{1.25}PRu$	
Color	pale green	
Formula weight	822.35 g · mol^{-1}	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	**$P2_1/c$, (no. 14)**	
Unit cell dimensions	a = 9.58710(10) Å	α= 90°.
	b = 23.6782(2) Å	β= 92.23°.
	c = 37.7484(4) Å	γ = 90°.
Volume	8562.60(15) Å^3	

Z	8	
Density (calculated)	1.276 $Mg \cdot m^{-3}$	
Absorption coefficient	0.562 mm^{-1}	
F(000)	3448 e	
Crystal size	0.14 x 0.12 x 0.04 mm^3	
θ range for data collection	3.74 to 26.79°.	
Index ranges	$-10 \le h \le 12$, $-29 \le k \le 29$, $-47 \le l \le 44$	
Reflections collected	36272	
Independent reflections	14072 [$R_{int} = 0.0569$]	
Reflections with $I>2\sigma(I)$	9594	
Completeness to $\theta = 26.79°$	76.9 %	
Absorption correction	Psi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14072 / 0 / 889	
Goodness-of-fit on F^2	1.021	
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0768$	$wR^2 = 0.1899$
R indices (all data)	$R_1 = 0.1210$	$wR^2 = 0.2157$
Largest diff. peak and hole	1.693 and -1.117 $e \cdot Å^{-3}$	

Table 10. X-ray structure analysis of complex 10. Atomic coordinates and equivalent isotropic displacement parameters (Å^2). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	0.0800(1)	0.7209(1)	0.0328(1)	0.024(1)
Cl(1)	0.3264(2)	0.7476(1)	0.0371(1)	0.017(1)
Cl(2)	0.1371(2)	0.6622(1)	0.0848(1)	0.020(1)
P(1)	0.0424(2)	0.8002(1)	-0.0039(1)	0.022(1)
C(1)	-0.1268(8)	0.7069(3)	0.0424(2)	0.027(2)
N(1)	-0.1897(7)	0.7286(2)	0.0712(2)	0.032(2)
C(2)	-0.3304(9)	0.7151(3)	0.0715(2)	0.035(2)
N(2)	-0.2339(6)	0.6759(2)	0.0256(2)	0.027(2)
C(3)	-0.3569(9)	0.6821(3)	0.0436(2)	0.037(2)
C(4)	-0.1267(9)	0.7660(4)	0.0982(2)	0.037(2)
C(5)	-0.1192(10)	0.7391(5)	0.1351(3)	0.055(3)
C(6)	-0.0991(13)	0.7846(6)	0.1649(3)	0.077(4)
O(7)	-0.0578(17)	0.7529(7)	0.1990(5)	0.132(5)
O(8)	0.0037(17)	0.8288(7)	0.1561(4)	0.133(5)
O(9)	-0.2326(12)	0.8137(5)	0.1691(3)	0.084(3)
C(7)	-0.0578(17)	0.7529(7)	0.1990(5)	0.132(5)
C(8)	0.0037(17)	0.8288(7)	0.1561(4)	0.133(5)
C(9)	-0.2326(12)	0.8137(5)	0.1691(3)	0.084(3)
C(11)	-0.2275(8)	0.6344(3)	-0.0022(2)	0.029(2)
C(12)	-0.1690(8)	0.5815(3)	0.0065(2)	0.031(2)
C(13)	-0.1708(8)	0.5409(3)	-0.0196(2)	0.033(2)
C(14)	-0.2276(9)	0.5498(3)	-0.0527(3)	0.042(2)
C(15)	-0.2913(9)	0.6021(3)	-0.0600(2)	0.037(2)
C(16)	-0.2935(8)	0.6445(3)	-0.0351(2)	0.034(2)
C(17)	-0.1076(9)	0.5695(3)	0.0430(2)	0.038(2)
C(18)	-0.2266(12)	0.5043(4)	-0.0817(3)	0.069(3)
C(19)	-0.3732(9)	0.6979(3)	-0.0441(3)	0.042(2)
C(20)	0.0719(8)	0.6742(3)	-0.0064(2)	0.025(2)
C(21)	0.1730(8)	0.6316(3)	-0.0163(2)	0.032(2)
C(22)	0.2895(8)	0.6153(3)	0.0050(3)	0.037(2)
C(23)	0.3863(9)	0.5773(3)	-0.0075(3)	0.042(2)
C(24)	0.3674(11)	0.5553(3)	-0.0419(3)	0.054(3)

C(25)	0.2529(10)	0.5700(3)	-0.0626(3)	0.045(2)
C(26)	0.1581(9)	0.6073(3)	-0.0499(2)	0.038(2)
C(31)	0.1361(8)	0.8614(3)	0.0176(2)	0.024(2)
C(32)	0.1225(8)	0.8652(3)	0.0575(2)	0.027(2)
C(33)	0.2228(9)	0.9083(3)	0.0736(2)	0.034(2)
C(34)	0.2050(9)	0.9664(3)	0.0563(2)	0.034(2)
C(35)	0.2129(8)	0.9633(3)	0.0167(2)	0.029(2)
C(36)	0.1101(8)	0.9202(3)	0.0007(2)	0.028(2)
C(41)	-0.1419(7)	0.8218(3)	-0.0139(2)	0.024(2)
C(42)	-0.1725(8)	0.8644(3)	-0.0444(2)	0.029(2)
C(43)	-0.3305(8)	0.8693(3)	-0.0518(2)	0.035(2)
C(44)	-0.4067(8)	0.8875(3)	-0.0190(2)	0.034(2)
C(45)	-0.3729(8)	0.8486(3)	0.0122(2)	0.031(2)
C(46)	-0.2151(8)	0.8437(3)	0.0194(2)	0.030(2)
C(51)	0.1177(8)	0.7992(3)	-0.0485(2)	0.024(2)
C(52)	0.0388(8)	0.7618(3)	-0.0759(2)	0.032(2)
C(53)	0.0947(9)	0.7714(4)	-0.1125(2)	0.042(2)
C(54)	0.2504(9)	0.7567(4)	-0.1131(2)	0.041(2)
C(55)	0.3313(9)	0.7907(3)	-0.0855(2)	0.035(2)
C(56)	0.2727(8)	0.7839(3)	-0.0492(2)	0.030(2)
Ru(1A)	-0.4018(1)	0.5463(1)	-0.2721(1)	0.035(1)
Cl(1A)	-0.3404(2)	0.6402(1)	-0.2489(1)	0.039(1)
Cl(2A)	-0.1584(2)	0.5443(1)	-0.2901(1)	0.029(1)
P(1A)	-0.4498(2)	0.4721(1)	-0.3121(1)	0.032(1)
C(1A)	-0.6044(10)	0.5685(3)	-0.2629(2)	0.040(2)
N(1A)	-0.6756(8)	0.6095(3)	-0.2817(2)	0.041(2)
C(2A)	-0.8035(11)	0.6203(4)	-0.2691(3)	0.059(3)
N(2A)	-0.6992(9)	0.5549(3)	-0.2372(2)	0.047(2)
C(3A)	-0.8196(12)	0.5858(4)	-0.2412(3)	0.061(3)
C(4A)	-0.6285(11)	0.6388(3)	-0.3132(2)	0.046(2)
C(5A)	-0.6050(11)	0.7016(3)	-0.3070(3)	0.050(3)
C(6A)	-0.5969(14)	0.7372(4)	-0.3418(4)	0.089(5)
O(7A)	-0.5251(15)	0.7933(6)	-0.3321(4)	0.114(4)
O(8A)	-0.5201(17)	0.7036(6)	-0.3697(5)	0.132(5)
O(9A)	-0.7481(16)	0.7495(6)	-0.3514(4)	0.121(5)
C(7A)	-0.5251(15)	0.7933(6)	-0.3321(4)	0.114(4)
C(8A)	-0.5201(17)	0.7036(6)	-0.3697(5)	0.132(5)
C(9A)	-0.7481(16)	0.7495(6)	-0.3514(4)	0.121(5)
C(11A)	-0.6723(11)	0.5203(4)	-0.2059(2)	0.047(2)

C(12A)	-0.7279(12)	0.4662(4)	-0.2042(3)	0.054(3)
C(13A)	-0.7009(11)	0.4353(4)	-0.1732(3)	0.054(3)
C(14A)	-0.6228(11)	0.4573(4)	-0.1447(2)	0.047(2)
C(15A)	-0.5807(11)	0.5122(4)	-0.1466(2)	0.048(2)
C(16A)	-0.6042(11)	0.5448(4)	-0.1767(3)	0.049(3)
C(17A)	-0.8176(12)	0.4405(4)	-0.2348(3)	0.061(3)
C(18A)	-0.5948(14)	0.4211(4)	-0.1124(3)	0.071(4)
C(19A)	-0.5565(13)	0.6054(4)	-0.1769(3)	0.062(3)
C(20A)	-0.3967(10)	0.4952(3)	-0.2347(2)	0.038(2)
C(21A)	-0.2877(10)	0.4855(4)	-0.2084(2)	0.040(2)
C(22A)	-0.2973(11)	0.4375(4)	-0.1867(2)	0.046(2)
C(23A)	-0.1960(13)	0.4228(4)	-0.1626(3)	0.061(3)
C(24A)	-0.0776(13)	0.4565(5)	-0.1577(3)	0.063(3)
C(25A)	-0.0682(11)	0.5058(5)	-0.1777(3)	0.060(3)
C(26A)	-0.1714(11)	0.5207(4)	-0.2025(3)	0.053(3)
C(31A)	-0.3732(9)	0.4010(3)	-0.3020(2)	0.040(2)
C(32A)	-0.2166(10)	0.4012(3)	-0.2923(3)	0.046(2)
C(33A)	-0.1606(11)	0.3403(4)	-0.2894(3)	0.054(3)
C(34A)	-0.2413(11)	0.3037(4)	-0.2641(3)	0.053(3)
C(35A)	-0.3960(11)	0.3059(3)	-0.2736(3)	0.052(3)
C(36A)	-0.4482(10)	0.3671(3)	-0.2733(2)	0.044(2)
C(41A)	-0.6349(9)	0.4537(3)	-0.3227(2)	0.035(2)
C(42A)	-0.6691(9)	0.3977(3)	-0.3424(2)	0.040(2)
C(43A)	-0.8248(10)	0.3863(4)	-0.3446(3)	0.051(3)
C(44A)	-0.9051(10)	0.4344(4)	-0.3624(3)	0.048(2)
C(45A)	-0.8729(10)	0.4902(4)	-0.3451(3)	0.050(2)
C(46A)	-0.7148(9)	0.5014(3)	-0.3427(2)	0.039(2)
C(51A)	-0.3670(10)	0.4895(3)	-0.3543(2)	0.037(2)
C(52A)	-0.3949(10)	0.4507(3)	-0.3859(2)	0.042(2)
C(53A)	-0.2947(11)	0.4637(3)	-0.4158(2)	0.044(2)
C(54A)	-0.3106(12)	0.5249(4)	-0.4277(2)	0.053(3)
C(55A)	-0.2861(12)	0.5652(4)	-0.3964(3)	0.057(3)
C(56A)	-0.3866(10)	0.5515(3)	-0.3664(2)	0.039(2)
C(100)	-0.169(2)	0.6618(7)	-0.1522(5)	0.047(5)
O(100)	-0.298(2)	0.7408(8)	-0.1364(6)	0.105(6)
C(101)	-0.233(3)	0.7155(10)	-0.1585(6)	0.070(8)
C(102)	-0.210(2)	0.7481(7)	-0.1926(5)	0.057(6)

Table 11. X-ray structure analysis of complex 10. Bond lengths [Å] and angles [°].

Ru(1)-C(20)	1.845(7)	Ru(1)-C(1)	2.057(8)
Ru(1)-P(1)	2.3520(18)	Ru(1)-Cl(1)	2.4444(16)
Ru(1)-Cl(2)	2.4507(16)	P(1)-C(51)	1.858(7)
P(1)-C(41)	1.864(7)	P(1)-C(31)	1.873(7)
C(1)-N(1)	1.365(10)	C(1)-N(2)	1.392(10)
N(1)-C(2)	1.387(10)	N(1)-C(4)	1.462(10)
C(2)-C(3)	1.331(12)	N(2)-C(3)	1.389(10)
N(2)-C(11)	1.443(10)	C(4)-C(5)	1.533(12)
C(5)-C(6)	1.563(16)	C(6)-O(9)	1.467(16)
C(6)-O(8)	1.484(19)	C(6)-O(7)	1.529(19)
C(11)-C(16)	1.393(12)	C(11)-C(12)	1.406(10)
C(12)-C(13)	1.377(11)	C(12)-C(17)	1.503(12)
C(13)-C(14)	1.360(12)	C(14)-C(15)	1.404(11)
C(14)-C(18)	1.536(12)	C(15)-C(16)	1.374(11)
C(16)-C(19)	1.509(10)	C(20)-C(21)	1.457(10)
C(21)-C(26)	1.396(12)	C(21)-C(22)	1.405(12)
C(22)-C(23)	1.389(11)	C(23)-C(24)	1.404(14)
C(24)-C(25)	1.367(14)	C(25)-C(26)	1.367(11)
C(31)-C(32)	1.521(10)	C(31)-C(36)	1.546(9)
CC(32)-C(33)	1.513(10)	C(33)-C(34)	1.528(10)
C(34)-C(35)	1.504(11)	C(35)-C(36)	1.527(10)
C(41)-C(46)	1.552(10)	C(41)-C(42)	1.553(10)
C(42)-C(43)	1.534(11)	C(43)-C(44)	1.524(11)
C(44)-C(45)	1.520(11)	C(45)-C(46)	1.531(10)
C(51)-C(56)	1.530(10)	C(51)-C(52)	1.539(10)
C(52)-C(53)	1.516(11)	C(53)-C(54)	1.534(12)
C(54)-C(55)	1.507(12)	C(55)-C(56)	1.509(11)
Ru(1A)-C(20A)	1.860(8)	Ru(1A)-C(1A)	2.056(9)
Ru(1A)-P(1A)	2.349(2)	Ru(1A)-Cl(1A)	2.4536(18)
Ru(1A)-Cl(2A)	2.455(2)	P(1A)-C(51A)	1.856(8)
P(1A)-C(41A)	1.856(9)	P(1A)-C(31A)	1.870(8)
C(1A)-N(1A)	1.369(11)	C(1A)-N(2A)	1.392(10)
N(1A)-C(2A)	1.357(12)	N(1A)-C(4A)	1.464(10)
C(2A)-C(3A)	1.346(13)	N(2A)-C(3A)	1.372(12)
N(2A)-C(11A)	1.451(11)	C(4A)-C(5A)	1.522(11)
C(5A)-C(6A)	1.565(16)	C(6A)-O(9A)	1.508(19)

C(6A)-O(8A)	1.531(19)	C(6A)-O(7A)	1.533(17)
C(11A)-C(16A)	1.385(13)	C(11A)-C(12A)	1.391(12)
C(12A)-C(13A)	1.398(13)	C(12A)-C(17A)	1.537(15)
C(13A)-C(14A)	1.388(14)	C(14A)-C(15A)	1.364(12)
C(14A)-C(18A)	1.504(13)	C(15A)-C(16A)	1.385(12)
C(16A)-C(19A)	1.506(12)	C(20A)-C(21A)	1.432(13)
C(21A)-C(26A)	1.403(13)	C(21A)-C(22A)	1.405(12)
C(22A)-C(23A)	1.350(14)	C(23A)-C(24A)	1.393(16)
C(24A)-C(25A)	1.395(15)	C(25A)-C(26A)	1.381(14)
C(31A)-C(32A)	1.532(12)	C(31A)-C(36A)	1.549(11)
C(32A)-C(33A)	1.541(11)	C(33A)-C(34A)	1.523(13)
C(34A)-C(35A)	1.514(14)	C(35A)-C(36A)	1.532(11)
C(41A)-C(46A)	1.546(11)	C(41A)-C(42A)	1.549(11)
C(42A)-C(43A)	1.516(12)	C(43A)-C(44A)	1.518(13)
C(44A)-C(45A)	1.500(13)	C(45A)-C(46A)	1.537(12)
C(51A)-C(52A)	1.520(11)	C(51A)-C(56A)	1.546(10)
C(52A)-C(53A)	1.541(12)	C(53A)-C(54A)	1.524(12)
C(54A)-C(55A)	1.528(13)	C(55A)-C(56A)	1.550(12)
C(100)-C(101)	1.43(3)		

C(20)-Ru(1)-C(1)	91.9(3)	C(20)-Ru(1)-P(1)	90.4(2)
C(1)-Ru(1)-P(1)	96.05(19)	C(20)-Ru(1)-Cl(1)	102.6(2)
C(1)-Ru(1)-Cl(1)	165.0(2)	P(1)-Ru(1)-Cl(1)	87.63(6)
C(20)-Ru(1)-Cl(2)	107.6(2)	C(1)-Ru(1)-Cl(2)	87.4(2)
P(1)-Ru(1)-Cl(2)	161.59(7)	Cl(1)-Ru(1)-Cl(2)	84.74(6)
C(51)-P(1)-C(41)	102.7(3)	C(51)-P(1)-C(31)	101.8(3)
C(41)-P(1)-C(31)	108.1(3)	C(51)-P(1)-Ru(1)	117.8(2)
C(41)-P(1)-Ru(1)	117.4(2)	C(31)-P(1)-Ru(1)	107.7(2)
N(1)-C(1)-N(2)	102.6(6)	N(1)-C(1)-Ru(1)	122.6(6)
N(2)-C(1)-Ru(1)	134.8(6)	C(1)-N(1)-C(2)	112.4(7)
C(1)-N(1)-C(4)	126.9(7)	C(2)-N(1)-C(4)	120.6(7)
C(3)-C(2)-N(1)	106.5(7)	C(3)-N(2)-C(1)	110.5(6)
C(3)-N(2)-C(11)	119.1(6)	C(1)-N(2)-C(11)	129.6(6)
C(2)-C(3)-N(2)	107.9(8)	N(1)-C(4)-C(5)	112.8(7)
C(4)-C(5)-C(6)	111.7(9)	O(9)-C(6)-O(8)	106.5(12)
O(9)-C(6)-O(7)	109.7(10)	O(8)-C(6)-O(7)	112.5(12)
O(9)-C(6)-C(5)	108.5(10)	O(8)-C(6)-C(5)	112.8(10)
O(7)-C(6)-C(5)	106.7(11)	C(16)-C(11)-C(12)	121.6(7)
C(16)-C(11)-N(2)	120.2(6)	C(12)-C(11)-N(2)	117.7(8)

C(13)-C(12)-C(11)	117.5(8)	C(13)-C(12)-C(17)	121.1(7)
C(11)-C(12)-C(17)	121.4(7)	C(14)-C(13)-C(12)	122.9(7)
C(13)-C(14)-C(15)	118.1(8)	C(13)-C(14)-C(18)	122.3(8)
C(15)-C(14)-C(18)	119.6(9)	C(16)-C(15)-C(14)	121.9(9)
C(15)-C(16)-C(11)	117.8(7)	C(15)-C(16)-C(19)	118.6(9)
C(11)-C(16)-C(19)	123.5(7)	C(21)-C(20)-Ru(1)	127.7(6)
C(26)-C(21)-C(22)	117.3(7)	C(26)-C(21)-C(20)	118.2(8)
C(22)-C(21)-C(20)	124.4(7)	C(23)-C(22)-C(21)	120.6(8)
C(22)-C(23)-C(24)	119.5(9)	C(25)-C(24)-C(23)	120.4(8)
C(24)-C(25)-C(26)	119.6(9)	C(25)-C(26)-C(21)	122.7(9)
C(32)-C(31)-C(36)	109.7(6)	C(32)-C(31)-P(1)	114.6(5)
C(36)-C(31)-P(1)	116.8(6)	C(33)-C(32)-C(31)	111.2(6)
C(32)-C(33)-C(34)	112.1(7)	C(35)-C(34)-C(33)	111.8(6)
C(34)-C(35)-C(36)	111.7(6)	C(35)-C(36)-C(31)	110.2(7)
C(46)-C(41)-C(42)	107.8(6)	C(46)-C(41)-P(1)	112.5(5)
C(42)-C(41)-P(1)	118.6(5)	C(43)-C(42)-C(41)	109.9(6)
C(44)-C(43)-C(42)	112.0(7)	C(45)-C(44)-C(43)	111.4(6)
C(44)-C(45)-C(46)	111.3(6)	C(45)-C(46)-C(41)	110.9(7)
C(56)-C(51)-C(52)	107.7(6)	C(56)-C(51)-P(1)	115.6(5)
C(52)-C(51)-P(1)	114.8(5)	C(53)-C(52)-C(51)	110.1(6)
C(52)-C(53)-C(54)	111.0(8)	C(55)-C(54)-C(53)	110.0(7)
C(54)-C(55)-C(56)	111.7(7)	C(55)-C(56)-C(51)	112.8(7)
C(20A)-Ru(1A)-C(1A)	92.0(4)	C(20A)-Ru(1A)-P(1A)	90.0(3)
C(1A)-Ru(1A)-P(1A)	97.9(2)	C(20A)-Ru(1A)-Cl(1A)	108.6(3)
C(1A)-Ru(1A)-Cl(1A)	85.6(2)	P(1A)-Ru(1A)-Cl(1A)	161.02(8)
C(20A)-Ru(1A)-Cl(2A)	101.5(3)	C(1A)-Ru(1A)-Cl(2A)	165.1(2)
P(1A)-Ru(1A)-Cl(2A)	88.46(7)	Cl(1A)-Ru(1A)-Cl(2A)	84.19(7)
C(51A)-P(1A)-C(41A)	107.7(4)	C(51A)-P(1A)-C(31A)	101.3(4)
C(41A)-P(1A)-C(31A)	101.4(4)	C(51A)-P(1A)-Ru(1A)	107.8(3)
C(41A)-P(1A)-Ru(1A)	118.4(3)	C(31A)-P(1A)-Ru(1A)	118.5(3)
N(1A)-C(1A)-N(2A)	101.6(7)	N(1A)-C(1A)-Ru(1A)	123.2(6)
N(2A)-C(1A)-Ru(1A)	134.9(7)	C(2A)-N(1A)-C(1A)	113.0(7)
C(2A)-N(1A)-C(4A)	120.4(8)	C(1A)-N(1A)-C(4A)	126.5(7)
C(3A)-C(2A)-N(1A)	107.0(9)	C(3A)-N(2A)-C(1A)	111.6(8)
C(3A)-N(2A)-C(11A)	121.0(8)	C(1A)-N(2A)-C(11A)	126.7(8)
C(2A)-C(3A)-N(2A)	106.9(9)	N(1A)-C(4A)-C(5A)	112.7(7)
C(4A)-C(5A)-C(6A)	114.1(9)	O(9A)-C(6A)-O(8A)	114.7(14)
O(9A)-C(6A)-O(7A)	108.0(10)	O(8A)-C(6A)-O(7A)	113.0(11)
O(9A)-C(6A)-C(5A)	103.1(10)	O(8A)-C(6A)-C(5A)	109.7(10)

O(7A)-C(6A)-C(5A)	107.7(12)	C(16A)-C(11A)-C(12A)	121.3(8)
C(16A)-C(11A)-N(2A)	118.3(8)	C(12A)-C(11A)-N(2A)	120.0(9)
C(11A)-C(12A)-C(13A)	117.5(10)	C(11A)-C(12A)-C(17A)	122.4(9)
C(13A)-C(12A)-C(17A)	120.1(9)	C(14A)-C(13A)-C(12A)	122.0(9)
C(15A)-C(14A)-C(13A)	117.8(8)	C(15A)-C(14A)-C(18A)	122.8(10)
C(13A)-C(14A)-C(18A)	119.2(9)	C(14A)-C(15A)-C(16A)	122.5(9)
C(15A)-C(16A)-C(11A)	118.3(8)	C(15A)-C(16A)-C(19A)	119.7(9)
C(11A)-C(16A)-C(19A)	122.0(8)	C(21A)-C(20A)-Ru(1A)	128.9(6)
C(26A)-C(21A)-C(22A)	117.3(10)	C(26A)-C(21A)-C(20A)	124.7(8)
C(22A)-C(21A)-C(20A)	118.1(9)	C(23A)-C(22A)-C(21A)	122.6(10)
C(22A)-C(23A)-C(24A)	120.2(10)	C(23A)-C(24A)-C(25A)	118.4(11)
C(26A)-C(25A)-C(24A)	121.4(11)	C(25A)-C(26A)-C(21A)	119.9(9)
C(32A)-C(31A)-C(36A)	108.1(7)	C(32A)-C(31A)-P(1A)	114.8(5)
C(36A)-C(31A)-P(1A)	114.8(6)	C(31A)-C(32A)-C(33A)	110.5(7)
C(34A)-C(33A)-C(32A)	113.0(7)	C(35A)-C(34A)-C(33A)	110.5(8)
C(34A)-C(35A)-C(36A)	110.4(8)	C(35A)-C(36A)-C(31A)	109.0(7)
C(46A)-C(41A)-C(42A)	107.4(7)	C(46A)-C(41A)-P(1A)	112.7(5)
C(42A)-C(41A)-P(1A)	119.2(6)	C(43A)-C(42A)-C(41A)	111.6(7)
C(42A)-C(43A)-C(44A)	111.8(7)	C(45A)-C(44A)-C(43A)	112.1(9)
C(44A)-C(45A)-C(46A)	111.3(8)	C(45A)-C(46A)-C(41A)	111.8(7)
C(52A)-C(51A)-C(56A)	109.1(7)	C(52A)-C(51A)-P(1A)	118.2(6)
C(56A)-C(51A)-P(1A)	114.4(5)	C(51A)-C(52A)-C(53A)	110.9(7)
C(54A)-C(53A)-C(52A)	110.3(7)	C(53A)-C(54A)-C(55A)	110.9(8)
C(54A)-C(55A)-C(56A)	110.6(8)	C(51A)-C(56A)-C(55A)	110.0(7)
O(100)-C(101)-C(100)	123(2)	O(100)-C(101)-C(102)	115(2)
C(100)-C(101)-C(102)	121.1(18)		

Table 12. X-ray structure analysis of complex 10. Anisotropic displacement parameters (Å^2). 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)	0.023(1)	0.022(1)	0.025(1)	0.004(1)	-0.002(1)	0.002(1)
Cl(1)	0.010(1)	0.016(1)	0.025(1)	0.003(1)	-0.005(1)	0.002(1)
Cl(2)	0.018(1)	0.026(1)	0.016(1)	0.015(1)	-0.001(1)	0.004(1)
P(1)	0.022(1)	0.019(1)	0.024(1)	0.002(1)	-0.003(1)	0.002(1)
C(1)	0.029(4)	0.024(3)	0.028(4)	0.010(3)	-0.002(4)	-0.002(3)
N(1)	0.035(4)	0.033(3)	0.028(4)	0.005(3)	0.003(4)	-0.002(3)
C(2)	0.026(4)	0.044(4)	0.035(5)	0.001(4)	0.002(5)	0.003(3)
N(2)	0.025(3)	0.022(3)	0.035(4)	0.000(2)	0.003(4)	0.000(2)
C(3)	0.032(5)	0.038(4)	0.041(5)	0.007(4)	0.007(5)	-0.001(3)
C(4)	0.034(5)	0.060(5)	0.018(4)	-0.001(3)	0.001(5)	-0.006(4)
C(5)	0.035(5)	0.099(8)	0.033(6)	0.006(5)	0.006(6)	0.012(5)
C(6)	0.065(8)	0.139(11)	0.027(6)	-0.004(6)	0.004(7)	0.009(8)
C(11)	0.024(4)	0.024(3)	0.039(5)	0.002(3)	-0.003(4)	-0.006(3)
C(12)	0.025(4)	0.023(3)	0.044(5)	0.004(3)	0.001(5)	0.000(3)
C(13)	0.027(4)	0.027(4)	0.045(5)	0.004(3)	-0.001(5)	0.004(3)
C(14)	0.040(5)	0.038(4)	0.046(6)	-0.007(4)	-0.008(5)	0.002(4)
C(15)	0.033(5)	0.034(4)	0.044(6)	0.001(3)	-0.009(5)	0.003(3)
C(16)	0.028(4)	0.024(4)	0.051(6)	0.002(3)	-0.003(5)	-0.004(3)
C(17)	0.043(5)	0.029(4)	0.041(5)	0.009(3)	0.001(5)	0.011(3)
C(18)	0.082(8)	0.043(5)	0.079(8)	-0.025(5)	-0.025(7)	0.019(5)
C(19)	0.046(5)	0.026(4)	0.053(6)	0.003(4)	-0.012(5)	0.005(4)
C(20)	0.025(4)	0.021(3)	0.027(4)	0.000(3)	-0.003(4)	-0.004(3)
C(21)	0.034(5)	0.019(3)	0.043(5)	0.001(3)	0.013(5)	-0.006(3)
C(22)	0.038(5)	0.021(3)	0.052(6)	0.004(3)	-0.001(5)	0.002(3)
C(23)	0.027(4)	0.030(4)	0.070(7)	0.006(4)	0.003(5)	0.003(3)
C(24)	0.049(6)	0.032(4)	0.084(8)	-0.011(5)	0.035(7)	-0.002(4)
C(25)	0.060(6)	0.031(4)	0.046(6)	-0.012(4)	0.020(6)	0.001(4)
C(26)	0.042(5)	0.025(4)	0.048(6)	-0.003(3)	-0.003(5)	-0.002(3)
C(31)	0.023(4)	0.020(3)	0.030(4)	-0.002(3)	0.003(4)	-0.002(3)
C(32)	0.032(4)	0.026(3)	0.024(4)	0.004(3)	-0.002(4)	-0.001(3)
C(33)	0.044(5)	0.034(4)	0.024(5)	-0.004(3)	-0.003(5)	-0.004(3)
C(34)	0.040(5)	0.027(4)	0.035(5)	-0.008(3)	-0.006(5)	-0.009(3)

C(35)	0.029(4)	0.021(3)	0.037(5)	-0.001(3)	-0.004(4)	0.000(3)
C(36)	0.029(4)	0.024(3)	0.032(5)	-0.003(3)	0.002(4)	0.004(3)
C(41)	0.025(4)	0.022(3)	0.024(4)	0.003(3)	-0.003(4)	-0.003(3)
C(42)	0.027(4)	0.027(3)	0.032(5)	0.002(3)	-0.008(4)	0.003(3)
C(43)	0.032(5)	0.032(4)	0.041(5)	0.005(3)	-0.011(5)	0.000(3)
C(44)	0.025(4)	0.026(4)	0.050(6)	-0.002(3)	-0.007(5)	0.003(3)
C(45)	0.024(4)	0.027(4)	0.042(5)	0.001(3)	-0.005(4)	-0.003(3)
C(46)	0.027(4)	0.026(3)	0.037(5)	0.001(3)	0.005(4)	0.001(3)
C(51)	0.028(4)	0.023(3)	0.021(4)	0.003(3)	-0.006(4)	-0.002(3)
C(52)	0.031(4)	0.031(4)	0.033(5)	-0.004(3)	-0.007(4)	0.001(3)
C(53)	0.043(5)	0.059(5)	0.024(5)	-0.004(4)	0.001(5)	-0.002(4)
C(54)	0.045(5)	0.049(5)	0.030(5)	0.000(4)	0.006(5)	0.006(4)
C(55)	0.031(5)	0.034(4)	0.039(5)	0.004(3)	0.003(5)	0.002(3)
C(56)	0.029(4)	0.028(4)	0.033(5)	-0.006(3)	0.000(4)	-0.004(3)
Ru(1A)	0.049(1)	0.031(1)	0.026(1)	0.002(1)	0.000(1)	-0.007(1)
Cl(1A)	0.053(1)	0.027(1)	0.036(1)	-0.004(1)	-0.002(1)	-0.014(1)
Cl(2A)	0.028(1)	0.040(1)	0.018(1)	0.001(1)	-0.001(1)	-0.006(1)
P(1A)	0.043(1)	0.030(1)	0.022(1)	0.002(1)	0.002(1)	-0.001(1)
C(1A)	0.062(6)	0.029(4)	0.029(5)	-0.003(3)	0.017(5)	-0.006(4)
N(1A)	0.050(5)	0.036(4)	0.039(5)	0.008(3)	0.017(4)	0.003(3)
C(2A)	0.061(7)	0.052(6)	0.064(8)	0.016(5)	0.014(7)	0.012(5)
N(2A)	0.056(5)	0.047(4)	0.039(5)	0.009(3)	0.017(5)	-0.007(4)
C(3A)	0.056(7)	0.067(6)	0.060(8)	0.016(5)	0.021(7)	0.010(5)
C(4A)	0.060(6)	0.041(5)	0.038(5)	0.008(4)	0.009(5)	0.005(4)
C(5A)	0.055(6)	0.035(4)	0.059(7)	0.007(4)	0.014(6)	0.001(4)
C(6A)	0.094(10)	0.046(6)	0.132(13)	0.010(7)	0.060(10)	-0.008(6)
C(11A)	0.065(7)	0.041(5)	0.036(6)	0.007(4)	0.014(6)	-0.001(4)
C(12A)	0.068(7)	0.052(5)	0.042(6)	0.007(4)	0.010(6)	-0.007(5)
C(13A)	0.071(7)	0.043(5)	0.050(7)	0.011(4)	0.038(6)	0.001(5)
C(14A)	0.064(7)	0.050(5)	0.029(5)	0.005(4)	0.014(6)	0.007(4)
C(15A)	0.062(7)	0.053(5)	0.030(5)	0.001(4)	0.012(5)	0.004(5)
C(16A)	0.070(7)	0.043(5)	0.035(6)	0.004(4)	0.014(6)	-0.003(4)
C(17A)	0.079(8)	0.061(6)	0.045(6)	0.002(5)	0.023(7)	-0.018(5)
C(18A)	0.107(10)	0.063(6)	0.044(7)	0.017(5)	0.018(7)	0.018(6)
C(19A)	0.091(9)	0.049(5)	0.048(7)	0.001(4)	0.007(7)	-0.013(5)
C(20A)	0.051(6)	0.037(4)	0.026(5)	0.006(3)	0.013(5)	-0.002(4)
C(21A)	0.047(6)	0.049(5)	0.025(5)	0.000(4)	-0.003(5)	0.007(4)
C(22A)	0.070(7)	0.044(5)	0.025(5)	0.004(4)	-0.003(5)	0.005(4)
C(23A)	0.091(9)	0.056(6)	0.035(6)	0.005(4)	-0.002(7)	0.008(6)

C(24A)	0.067(8)	0.087(8)	0.034(6)	0.004(5)	-0.009(7)	0.019(6)
C(25A)	0.041(6)	0.106(9)	0.032(6)	0.007(5)	-0.003(6)	-0.006(6)
C(26A)	0.066(7)	0.057(6)	0.036(6)	0.005(4)	0.006(6)	-0.015(5)
C(31A)	0.049(6)	0.030(4)	0.042(5)	-0.002(3)	-0.002(5)	0.001(4)
C(32A)	0.057(6)	0.041(5)	0.038(6)	0.003(4)	0.000(5)	0.008(4)
C(33A)	0.064(7)	0.045(5)	0.054(7)	0.000(4)	0.009(6)	0.015(5)
C(34A)	0.068(7)	0.051(5)	0.039(6)	0.008(4)	0.005(6)	0.022(5)
C(35A)	0.075(8)	0.037(5)	0.045(6)	0.006(4)	-0.001(6)	0.003(5)
C(36A)	0.060(6)	0.038(4)	0.033(5)	0.008(3)	0.000(5)	-0.003(4)
C(41A)	0.044(5)	0.038(4)	0.023(4)	0.000(3)	0.006(5)	-0.001(4)
C(42A)	0.048(6)	0.037(4)	0.034(5)	0.003(3)	0.004(5)	-0.005(4)
C(43A)	0.059(6)	0.055(5)	0.038(6)	0.001(4)	0.003(6)	-0.018(5)
C(44A)	0.039(5)	0.071(6)	0.035(6)	-0.001(4)	0.000(5)	-0.009(5)
C(45A)	0.051(6)	0.070(6)	0.030(5)	0.001(4)	-0.002(6)	0.004(5)
C(46A)	0.041(5)	0.043(4)	0.033(5)	-0.001(3)	-0.002(5)	0.004(4)
C(51A)	0.052(6)	0.029(4)	0.029(5)	0.001(3)	0.002(5)	-0.001(4)
C(52A)	0.056(6)	0.035(4)	0.036(5)	-0.003(3)	0.006(5)	-0.002(4)
C(53A)	0.062(6)	0.044(5)	0.027(5)	-0.006(3)	0.005(5)	-0.009(4)
C(54A)	0.079(8)	0.044(5)	0.035(6)	-0.001(4)	0.013(6)	-0.009(5)
C(55A)	0.084(8)	0.038(5)	0.051(7)	0.003(4)	0.017(6)	-0.010(5)
C(56A)	0.058(6)	0.034(4)	0.026(5)	0.002(3)	0.004(5)	-0.001(4)
C(100)	0.053(12)	0.049(10)	0.037(11)	-0.002(8)	-0.029(11)	-0.029(9)
O(100)	0.093(14)	0.111(15)	0.113(18)	0.001(12)	0.019(14)	-0.016(11)
C(101)	0.069(15)	0.090(17)	0.051(14)	-0.048(13)	0.023(14)	-0.058(13)
C(102)	0.069(14)	0.041(10)	0.057(14)	-0.024(9)	-0.044(13)	-0.007(9)

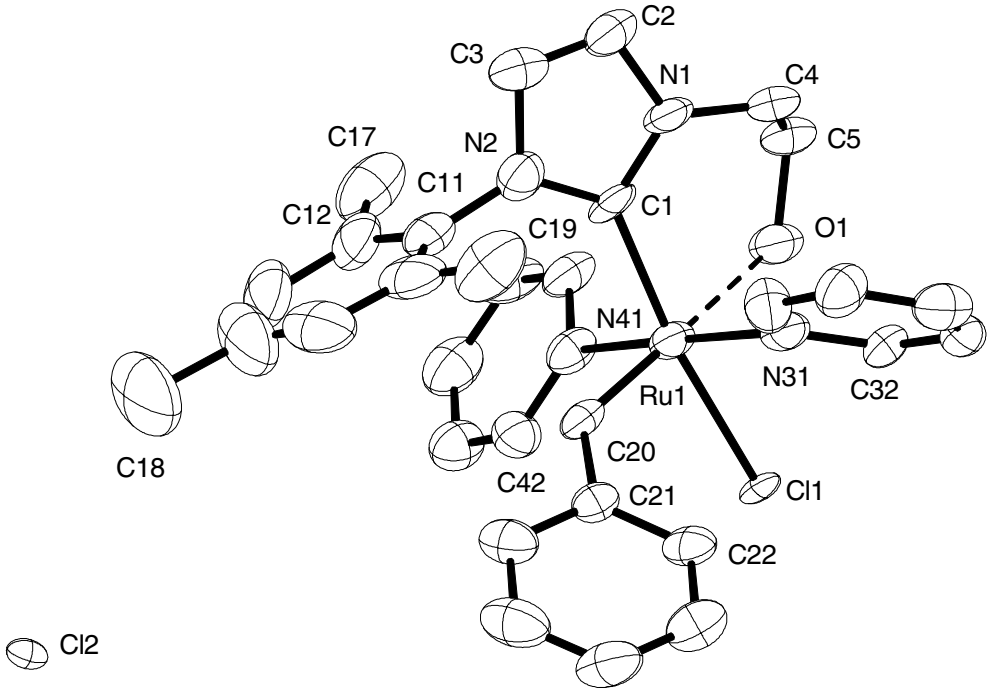

Figure 4. Molecular structure of complex **13** in the solid state. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are drawn at 50% probability.

Table 13. X-ray structure analysis of complex 13. Crystal data and structure refinement.

Empirical formula	$C_{36}H_{37}Cl_2N_4O_{3.50}Ru$	
Color	blue-violet	
Formula weight	753.67 $g \cdot mol^{-1}$	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	**Pbca, (no. 61)**	
Unit cell dimensions	a = 16.1863(3) Å	α= 90°.
	b = 14.7148(2) Å	β= 90°.
	c = 31.8092(5) Å	γ = 90°.
Volume	7576.3(2) $Å^3$	
Z	8	
Density (calculated)	1.321 $Mg \cdot m^{-3}$	
Absorption coefficient	0.594 mm^{-1}	
F(000)	3096 e	

Crystal size	0.17 x 0.15 x 0.07 mm^3	
θ range for data collection	4.21 to 23.26°.	
Index ranges	$-17 \le h \le 17$, $-16 \le k \le 16$, $-34 \le l \le 35$	
Reflections collected	16723	
Independent reflections	5210 [$R_{int} = 0.0708$]	
Reflections with $I>2\sigma(I)$	3750	
Completeness to $\theta = 23.26°$	95.8 %	
Absorption correction	Psi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5210 / 0 / 436	
Goodness-of-fit on F^2	1.071	
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0871$	$wR^2 = 0.2223$
R indices (all data)	$R_1 = 0.1217$	$wR^2 = 0.2447$
Largest diff. peak and hole	1.665 and -1.013 e · $Å^{-3}$	

Table 14. X-ray structure analysis of complex 13. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$). U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	0.1025(1)	0.3324(1)	0.1794(1)	0.035(1)
Cl(1)	0.1500(1)	0.1922(1)	0.2151(1)	0.025(1)
Cl(2)	0.1091(1)	0.1870(1)	-0.1661(1)	0.023(1)
C(1)	0.0653(7)	0.4591(6)	0.1588(3)	0.040(3)
N(2)	0.0713(5)	0.5021(6)	0.1215(3)	0.045(2)
C(3)	0.0347(7)	0.5906(7)	0.1239(4)	0.050(3)
C(2)	0.0071(7)	0.5999(7)	0.1633(4)	0.047(3)
N(1)	0.0250(5)	0.5188(5)	0.1845(3)	0.041(2)
C(4)	0.0040(8)	0.5049(7)	0.2285(4)	0.052(3)
C(5)	0.0779(9)	0.4845(7)	0.2552(4)	0.057(3)
O(1)	0.1108(5)	0.3976(5)	0.2449(2)	0.047(2)
C(11)	0.1086(8)	0.4744(8)	0.0822(4)	0.053(3)
C(12)	0.1928(9)	0.4959(9)	0.0751(4)	0.066(4)
C(13)	0.2232(13)	0.4712(12)	0.0358(6)	0.102(6)
C(14)	0.1775(18)	0.4291(16)	0.0052(6)	0.119(9)

C(15)	0.0961(15)	0.4134(11)	0.0138(5)	0.093(6)
C(16)	0.0589(11)	0.4335(9)	0.0524(4)	0.072(4)
C(17)	0.2466(9)	0.5482(11)	0.1070(5)	0.082(5)
C(18)	0.212(2)	0.4063(17)	-0.0391(6)	0.182(13)
C(19)	-0.0321(10)	0.4136(10)	0.0606(5)	0.078(4)
C(20)	0.1021(6)	0.2809(6)	0.1258(3)	0.034(2)
C(21)	0.0639(7)	0.1998(7)	0.1076(3)	0.039(3)
C(22)	0.0183(7)	0.1360(7)	0.1306(3)	0.040(3)
C(23)	-0.0151(7)	0.0600(8)	0.1115(4)	0.050(3)
C(24)	-0.0019(8)	0.0452(8)	0.0694(4)	0.060(4)
C(25)	0.0434(9)	0.1073(9)	0.0460(4)	0.066(4)
C(26)	0.0757(7)	0.1845(8)	0.0651(4)	0.050(3)
N(31)	-0.0204(5)	0.2994(6)	0.1935(3)	0.040(2)
C(32)	-0.0401(7)	0.2633(7)	0.2320(3)	0.044(3)
C(33)	-0.1186(7)	0.2455(7)	0.2440(4)	0.043(3)
C(34)	-0.1836(7)	0.2653(8)	0.2172(4)	0.054(3)
C(35)	-0.1644(7)	0.3026(8)	0.1784(4)	0.053(3)
C(36)	-0.0839(7)	0.3160(8)	0.1683(4)	0.047(3)
N(41)	0.2300(5)	0.3622(6)	0.1725(3)	0.040(2)
C(42)	0.2815(6)	0.3075(8)	0.1515(3)	0.044(3)
C(43)	0.3646(7)	0.3223(8)	0.1492(4)	0.050(3)
C(44)	0.3985(8)	0.3974(9)	0.1699(4)	0.062(4)
C(45)	0.3470(7)	0.4534(8)	0.1926(4)	0.055(3)
C(46)	0.2623(7)	0.4348(7)	0.1928(4)	0.049(3)
O(91)	-0.2104(14)	0.5421(14)	0.1903(11)	0.127(11)
C(92)	-0.268(2)	0.5610(17)	0.1531(7)	0.078(10)
C(93)	-0.291(2)	0.473(2)	0.1304(9)	0.100(12)
O(94)	0.0294(7)	0.7416(7)	0.0497(4)	0.087(3)
C(95)	0.0960(9)	0.7921(11)	0.0319(5)	0.078(4)
C(96)	0.1730(10)	0.7341(10)	0.0369(5)	0.085(5)
O(97)	0.1100(9)	0.1559(8)	-0.0664(4)	0.107(4)
C(98)	0.1747(9)	0.158(2)	-0.0564(8)	0.184(16)
C(99)	0.2537(14)	0.164(3)	-0.0688(7)	0.205(16)

Table 15. X-ray structure analysis of complex 13. Bond lengths [Å] and angles [°].

Ru(1)-C(20)	1.866(10)	Ru(1)-C(1)	2.067(10)
Ru(1)-N(31)	2.096(9)	Ru(1)-N(41)	2.121(8)
Ru(1)-O(1)	2.297(7)	Ru(1)-Cl(1)	2.477(2)
C(1)-N(2)	1.348(13)	C(1)-N(1)	1.365(13)
N(2)-C(3)	1.433(14)	N(2)-C(11)	1.446(15)
C(3)-C(2)	1.337(16)	C(2)-N(1)	1.401(13)
N(1)-C(4)	1.455(14)	C(4)-C(5)	1.497(17)
C(5)-O(1)	1.424(13)	C(11)-C(16)	1.381(19)
C(11)-C(12)	1.418(18)	C(12)-C(13)	1.39(2)
C(12)-C(17)	1.55(2)	C(13)-C(14)	1.37(3)
C(14)-C(15)	1.37(3)	C(14)-C(18)	1.55(2)
C(15)-C(16)	1.40(2)	C(16)-C(19)	1.52(2)
C(20)-C(21)	1.465(14)	C(21)-C(26)	1.384(15)
C(21)-C(22)	1.401(15)	C(22)-C(23)	1.383(15)
C(23)-C(24)	1.376(17)	C(24)-C(25)	1.386(18)
C(25)-C(26)	1.390(17)	N(31)-C(36)	1.326(14)
N(31)-C(32)	1.373(13)	C(32)-C(33)	1.353(15)
C(33)-C(34)	1.386(16)	C(34)-C(35)	1.387(17)
C(35)-C(36)	1.357(16)	N(41)-C(42)	1.336(13)
N(41)-C(46)	1.354(14)	C(42)-C(43)	1.365(15)
C(43)-C(44)	1.398(17)	C(44)-C(45)	1.377(18)
C(45)-C(46)	1.397(16)	O(91)-C(92)	1.54(4)
C(92)-C(93)	1.52(4)	O(94)-C(95)	1.427(16)
C(95)-C(96)	1.520(19)	O(97)-C(98)	1.095(18)
OC(98)-C(99)	1.34(3)		
C(20)-Ru(1)-C(1)	94.3(4)	C(20)-Ru(1)-N(31)	95.6(4)
C(1)-Ru(1)-N(31)	90.0(4)	C(20)-Ru(1)-N(41)	89.5(4)
C(1)-Ru(1)-N(41)	93.7(4)	N(31)-Ru(1)-N(41)	173.4(3)
C(20)-Ru(1)-O(1)	176.7(4)	C(1)-Ru(1)-O(1)	85.9(4)
N(31)-Ru(1)-O(1)	87.6(3)	N(41)-Ru(1)-O(1)	87.2(3)
C(20)-Ru(1)-Cl(1)	94.7(3)	C(1)-Ru(1)-Cl(1)	170.9(3)
N(31)-Ru(1)-Cl(1)	90.2(2)	N(41)-Ru(1)-Cl(1)	85.3(2)
O(1)-Ru(1)-Cl(1)	85.02(18)	N(2)-C(1)-N(1)	105.1(9)
N(2)-C(1)-Ru(1)	132.9(8)	N(1)-C(1)-Ru(1)	122.0(7)
C(1)-N(2)-C(3)	110.4(9)	C(1)-N(2)-C(11)	131.2(9)

C(3)-N(2)-C(11)	118.4(9)	C(2)-C(3)-N(2)	106.4(10)
C(3)-C(2)-N(1)	107.1(10)	C(1)-N(1)-C(2)	111.0(9)
C(1)-N(1)-C(4)	126.6(9)	C(2)-N(1)-C(4)	122.3(9)
N(1)-C(4)-C(5)	112.8(10)	C(5)-O(1)-Ru(1)	124.2(7)
C(16)-C(11)-C(12)	123.3(13)	C(16)-C(11)-N(2)	118.1(12)
C(12)-C(11)-N(2)	118.4(12)	C(13)-C(12)-C(11)	115.2(16)
C(13)-C(12)-C(17)	121.5(16)	C(11)-C(12)-C(17)	123.3(12)
C(14)-C(13)-C(12)	124.3(19)	C(15)-C(14)-C(13)	117.2(17)
C(15)-C(14)-C(18)	119(3)	C(13)-C(14)-C(18)	123(3)
C(14)-C(15)-C(16)	123.7(18)	C(11)-C(16)-C(15)	116.3(17)
C(11)-C(16)-C(19)	122.0(13)	C(15)-C(16)-C(19)	121.7(15)
C(21)-C(20)-Ru(1)	133.9(8)	C(26)-C(21)-C(22)	118.4(10)
C(26)-C(21)-C(20)	117.4(10)	C(22)-C(21)-C(20)	124.2(10)
C(23)-C(22)-C(21)	121.2(11)	C(24)-C(23)-C(22)	119.6(12)
C(23)-C(24)-C(25)	120.1(12)	C(24)-C(25)-C(26)	120.3(12)
C(21)-C(26)-C(25)	120.4(12)	C(36)-N(31)-C(32)	115.5(10)
C(36)-N(31)-Ru(1)	124.3(7)	C(32)-N(31)-Ru(1)	120.1(7)
C(33)-C(32)-N(31)	123.1(11)	C(32)-C(33)-C(34)	119.9(11)
C(33)-C(34)-C(35)	117.4(11)	C(36)-C(35)-C(34)	119.0(11)
N(31)-C(36)-C(35)	125.1(11)	C(42)-N(41)-C(46)	118.1(9)
C(42)-N(41)-Ru(1)	122.3(7)	C(46)-N(41)-Ru(1)	119.3(8)
N(41)-C(42)-C(43)	123.1(11)	C(42)-C(43)-C(44)	119.1(12)
C(45)-C(44)-C(43)	118.8(12)	C(44)-C(45)-C(46)	118.6(12)
N(41)-C(46)-C(45)	122.2(11)	C(93)-C(92)-O(91)	111(2)
O(94)-C(95)-C(96)	106.6(11)	O(97)-C(98)-C(99)	146(3)

Table 16. X-ray structure analysis of complex 13. Anisotropic displacement parameters (Å^2). 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)	0.040(1)	0.023(1)	0.043(1)	0.002(1)	0.001(1)	-0.003(1)
Cl(1)	0.034(1)	0.011(1)	0.030(1)	0.003(1)	-0.006(1)	-0.006(1)
Cl(2)	0.018(1)	0.020(1)	0.030(1)	-0.007(1)	-0.001(1)	0.003(1)
C(1)	0.052(7)	0.016(5)	0.051(7)	0.008(5)	0.000(5)	-0.013(5)
N(2)	0.045(5)	0.039(5)	0.053(6)	0.007(5)	0.005(4)	-0.005(4)
C(3)	0.053(7)	0.031(6)	0.067(9)	-0.001(6)	-0.005(6)	0.000(5)
C(2)	0.045(7)	0.032(6)	0.065(8)	0.012(5)	0.001(6)	-0.003(5)
N(1)	0.046(5)	0.018(4)	0.060(6)	0.007(4)	0.006(4)	0.000(4)
C(4)	0.073(8)	0.020(5)	0.063(8)	-0.001(5)	0.013(7)	0.002(6)
C(5)	0.084(10)	0.022(6)	0.063(8)	-0.005(5)	0.011(7)	-0.004(6)
O(1)	0.062(5)	0.028(4)	0.051(5)	0.000(3)	-0.001(4)	0.004(4)
C(11)	0.074(9)	0.034(6)	0.052(7)	0.013(6)	0.002(7)	0.010(6)
C(12)	0.077(10)	0.056(8)	0.066(9)	0.031(7)	0.017(8)	0.013(8)
C(13)	0.123(15)	0.093(13)	0.089(13)	0.056(11)	0.052(12)	0.045(12)
C(14)	0.17(2)	0.128(18)	0.057(12)	0.035(11)	0.037(14)	0.083(17)
C(15)	0.171(19)	0.064(10)	0.045(9)	0.008(7)	-0.015(11)	0.052(12)
C(16)	0.131(14)	0.037(7)	0.050(8)	0.008(6)	-0.015(9)	0.024(8)
C(17)	0.052(8)	0.072(10)	0.123(13)	0.039(9)	-0.006(9)	-0.003(7)
C(18)	0.32(3)	0.17(2)	0.064(12)	0.045(13)	0.072(16)	0.12(2)
C(19)	0.091(11)	0.073(10)	0.070(10)	0.019(8)	-0.038(8)	-0.016(9)
C(20)	0.035(5)	0.023(5)	0.045(6)	0.011(4)	-0.001(5)	-0.001(4)
C(21)	0.045(6)	0.030(6)	0.041(6)	0.008(5)	-0.001(5)	0.010(5)
C(22)	0.051(7)	0.030(6)	0.040(6)	0.002(5)	-0.012(5)	0.011(5)
C(23)	0.046(7)	0.041(7)	0.063(8)	0.004(6)	-0.018(6)	-0.008(6)
C(24)	0.086(10)	0.035(7)	0.061(9)	-0.003(6)	-0.018(7)	0.002(7)
C(25)	0.087(10)	0.058(9)	0.052(8)	-0.017(7)	-0.017(7)	0.022(8)
C(26)	0.055(7)	0.043(7)	0.051(7)	-0.006(6)	-0.008(6)	0.013(6)
N(31)	0.046(5)	0.025(4)	0.050(6)	0.000(4)	0.002(5)	-0.001(4)
C(32)	0.056(7)	0.026(6)	0.049(7)	0.005(5)	0.010(6)	-0.008(5)
C(33)	0.045(7)	0.030(6)	0.055(7)	-0.001(5)	0.014(6)	-0.004(5)
C(34)	0.033(6)	0.039(7)	0.091(10)	-0.007(7)	0.009(6)	-0.005(5)
C(35)	0.044(7)	0.048(7)	0.066(8)	0.010(6)	0.004(6)	-0.004(6)

C(36)	0.044(7)	0.057(8)	0.042(6)	0.005(5)	0.003(5)	0.004(6)
N(41)	0.031(5)	0.034(5)	0.055(6)	0.009(4)	-0.005(4)	-0.005(4)
C(42)	0.039(6)	0.041(6)	0.053(7)	-0.001(5)	0.006(5)	0.002(5)
C(43)	0.044(7)	0.044(7)	0.062(8)	0.002(6)	-0.001(6)	-0.002(6)
C(44)	0.044(7)	0.056(8)	0.086(10)	0.021(7)	-0.003(7)	0.002(7)
C(45)	0.052(8)	0.029(6)	0.085(9)	0.004(6)	-0.010(7)	-0.008(6)
C(46)	0.055(8)	0.028(6)	0.063(8)	0.010(5)	0.000(6)	-0.006(6)
O(91)	0.060(13)	0.048(12)	0.27(4)	-0.032(18)	-0.005(18)	0.023(11)
C(92)	0.16(3)	0.052(16)	0.024(12)	-0.013(11)	0.018(16)	0.026(19)
C(93)	0.15(3)	0.10(3)	0.058(18)	0.008(18)	0.002(19)	0.04(2)
O(94)	0.086(8)	0.084(7)	0.093(8)	0.028(6)	-0.012(6)	0.000(6)
C(95)	0.070(9)	0.068(9)	0.096(11)	0.031(9)	0.007(8)	0.001(8)
C(96)	0.098(12)	0.063(10)	0.093(11)	0.018(8)	0.004(9)	-0.003(9)
O(97)	0.124(11)	0.085(8)	0.114(10)	-0.005(8)	0.016(8)	0.009(8)
C(98)	0.018(8)	0.34(4)	0.19(2)	-0.14(2)	0.046(11)	-0.013(14)
C(99)	0.108(17)	0.40(5)	0.104(16)	-0.06(2)	0.002(14)	0.07(2)