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Supporting Information

Ruthenium(IV)–Bis(methallyl) Complexes as UV-Latent Initiators for Ring-Opening Metathesis Polymerization

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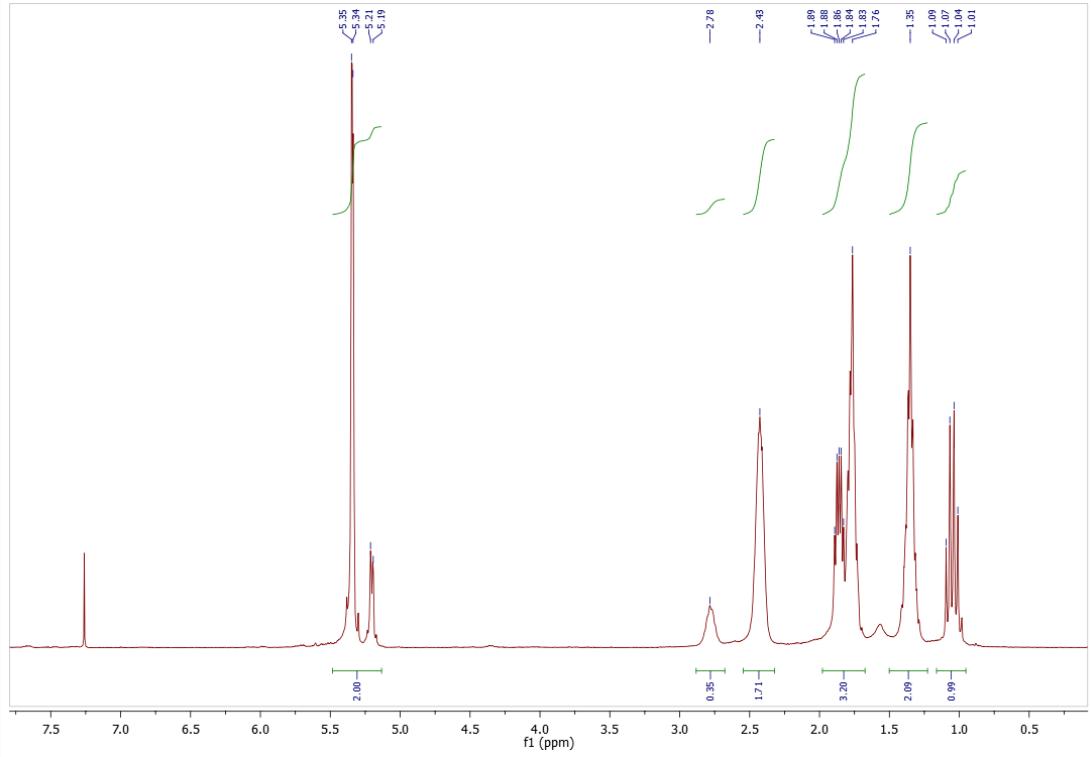


Figure **S13.** ^{1}H NMR spectrum ($CDCl_3$) of poly(NBE) prepared by **pre-catalyst 1**.

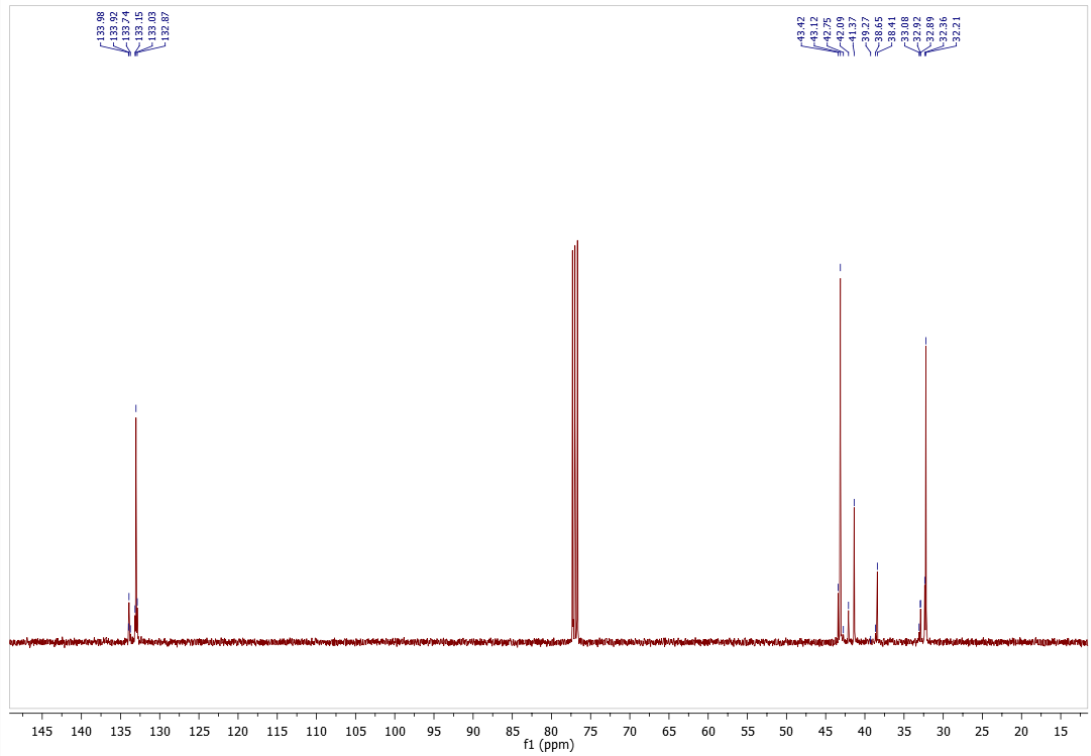


Figure **S14.** ^{13}C NMR spectrum ($CDCl_3$) of poly(NBE) prepared by **pre-catalyst 1**.

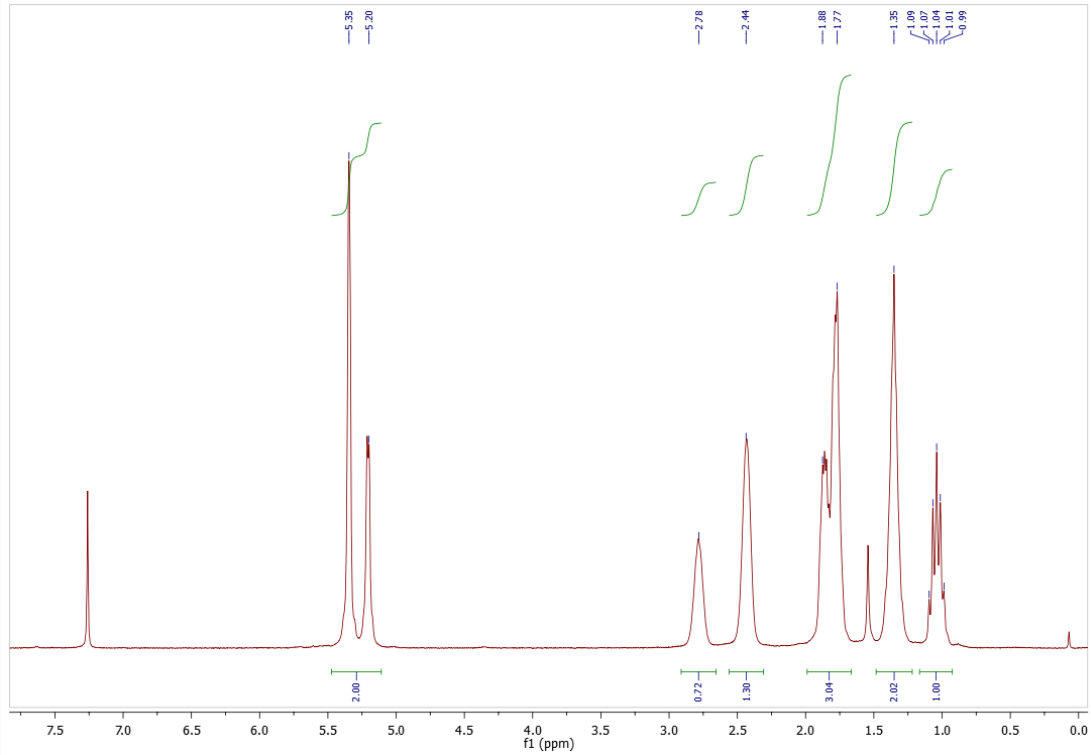


Figure **S15.** ^{1}H NMR spectrum ($CDCl_3$) of poly(NBE) prepared by **pre-catalyst 3**.

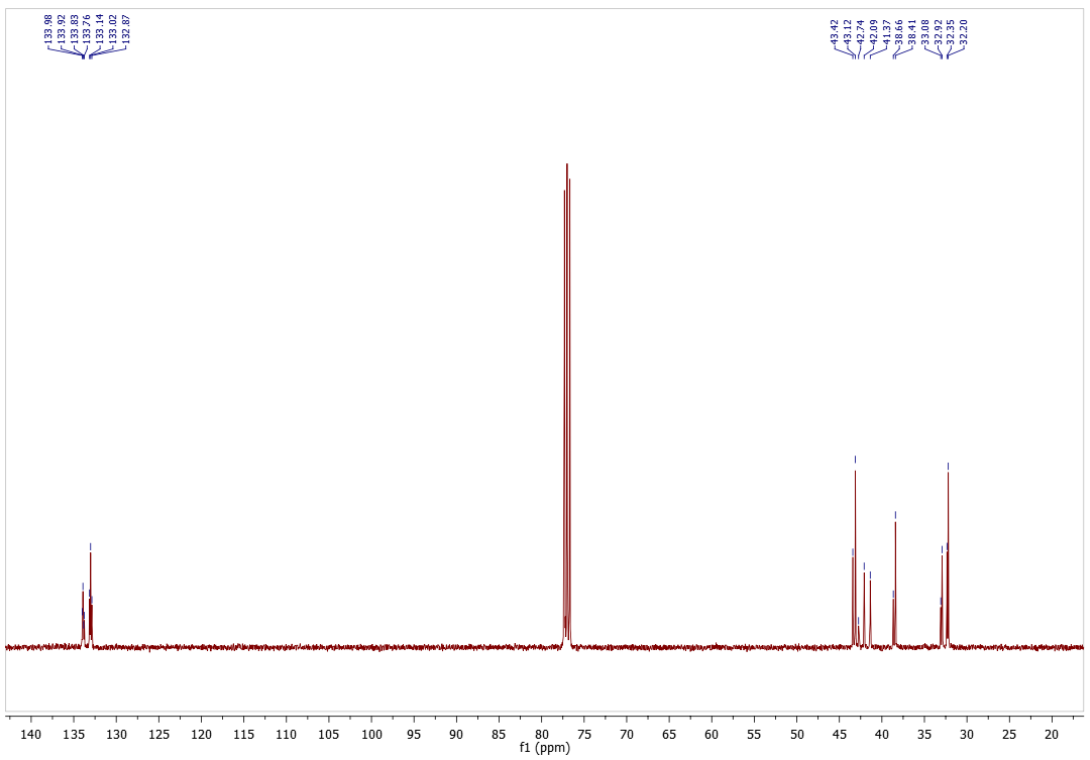
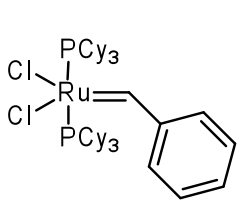


Figure **S16.** ^{13}C NMR spectrum ($CDCl_3$) of poly(NBE) prepared by **pre-catalyst 3**.



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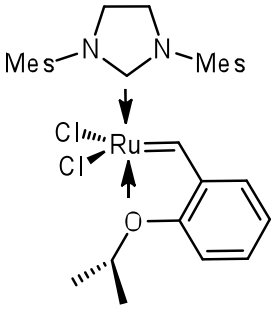

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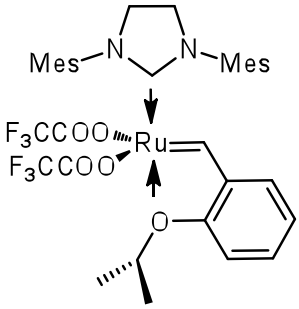

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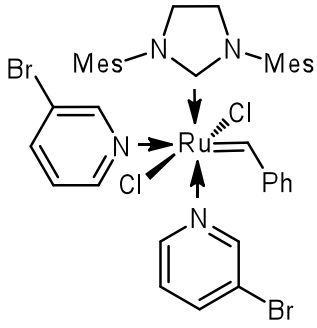

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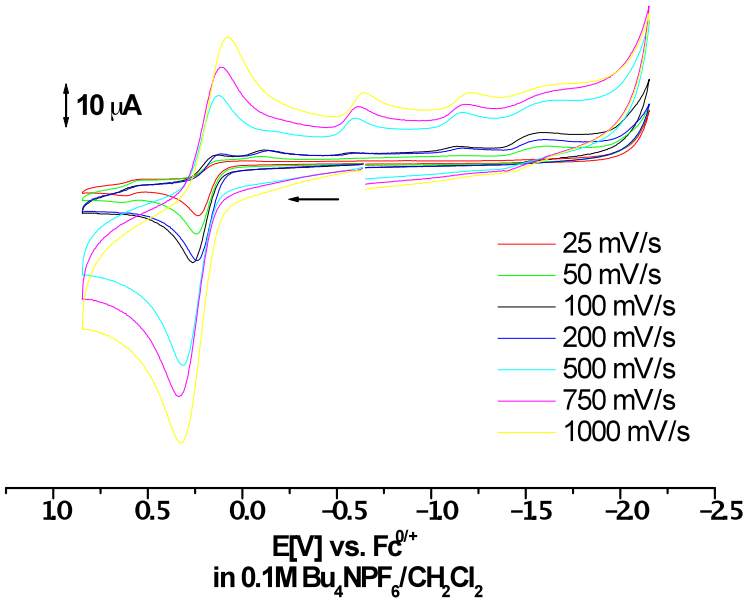

Figure S17: Cyclic voltammogram of **4** in CH_2Cl_2/0.1 M Bu_4NPF_6 at 295 K. The ferrocene/ferrocenium couple was used as an internal standard.

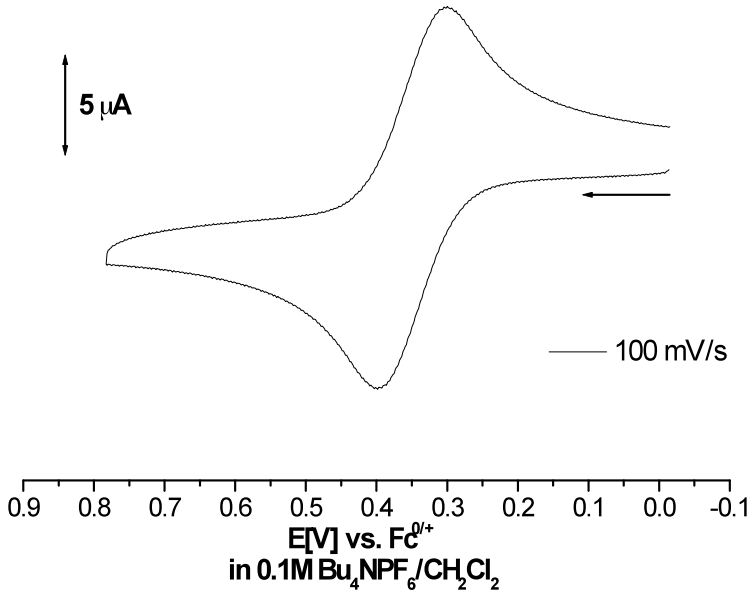

Figure S18: Cyclic voltammogram of **5** in CH_2Cl_2/0.1 M Bu_4NPF_6 at 295 K. Scan rate: 100 mV/s. The ferrocene/ferrocenium couple was used as an internal standard.

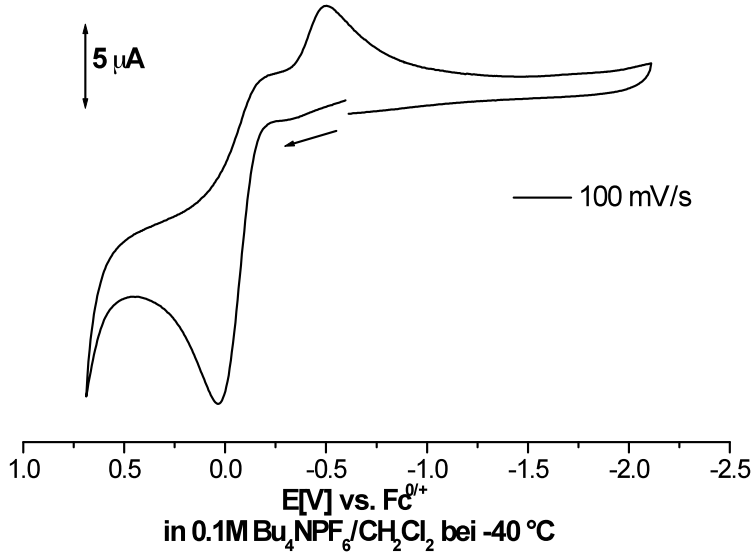

Figure S19: Cyclic voltammogram of **6** in CH_2Cl_2/0.1 M Bu_4NPF_6 at 233 K. Scan rate: 100 mV/s. The ferrocene/ferrocenium couple was used as an internal standard.

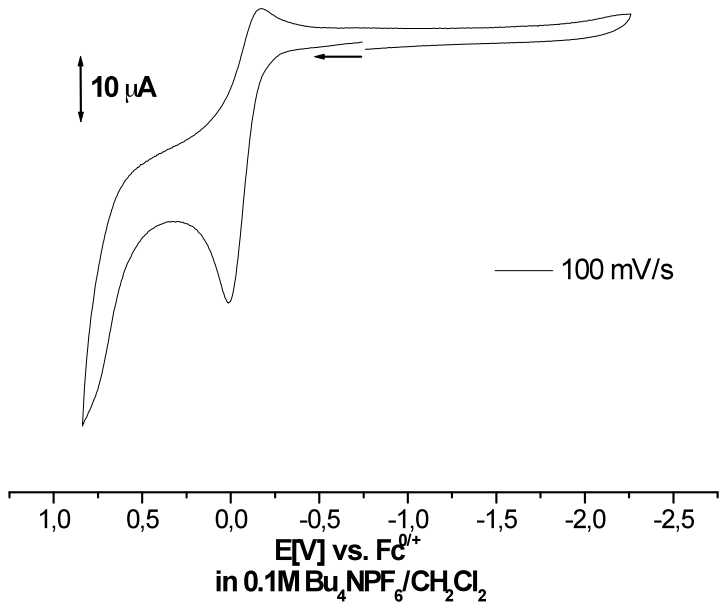

Figure S20: Cyclic voltammogram of **6** in CH_2Cl_2/0.1 M Bu_4NPF_6 at 295K. Scan rate: 100 mV/s. The ferrocene/ferrocenium couple was used as an internal standard.

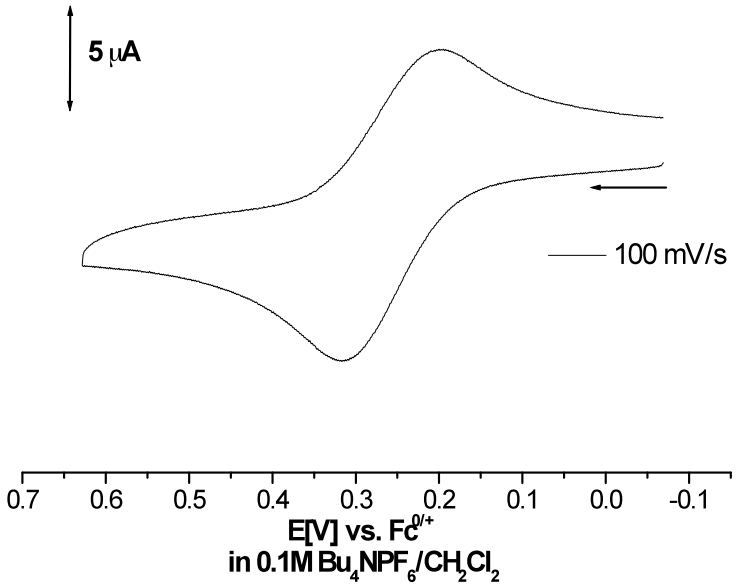

Figure S21. Cyclic voltammogram of **7** in CH_2Cl_2/0.1 M Bu_4NPF_6 at 295 K. Scan rate: 100 mV/s. The ferrocene/ferrocenium couple was used as an internal standard.

Table S1. Crystal data and structure refinement for [{Ru(η^3: η^3-$C_{10}H_{16}$)Cl_2(PPh_3)]•CH_2Cl_2 (**1**).

Empirical formula	C_{29} H_{33} Cl_4 P Ru	
Formula weight	655.39	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P 21/c	
Unit cell dimensions	a = 16.1262(7) Å	α = 90°.
	b = 9.4714(4) Å	β= 113.085(2)°.
	c = 19.9310(8) Å	γ= 90°.
Volume	2800.4(2) $Å^3$	
Z, Calculated density	4, 1.554 Mg/m^3	
Absorption coefficient	1.016 mm^{-1}	
F(000)	1336	
Crystal size	0.77 x 0.31 x 0.22 mm	
Theta range for data collection	2.10 to 33.28 °.	
Limiting indices	-24<=h<=24, -14<=k<=14, -30<=l<=30	
Reflections collected / unique	39108 / 10637 [R(int) = 0.0288]	
Completeness to theta = 33.28	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8073 and 0.5083	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10637 / 2 / 360	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0261, wR2 = 0.0645	
R indices (all data)	R1 = 0.0387, wR2 = 0.0731	
Largest diff. peak and hole	1.034 and -0.950 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	3935(1)	2177(1)	3338(1)	10(1)
Cl(1)	3202(1)	3030(1)	4112(1)	16(1)
Cl(2)	4561(1)	1308(1)	2494(1)	12(1)
C(1)	3538(1)	4041(2)	2623(1)	15(1)
C(2)	4202(1)	4533(2)	3287(1)	16(1)
C(3)	5033(1)	3833(2)	3526(1)	16(1)
C(4)	5776(1)	3978(2)	4274(1)	21(1)
C(5)	5992(1)	2473(2)	4567(1)	20(1)
C(6)	5089(1)	1795(2)	4427(1)	15(1)
C(7)	4808(1)	467(2)	4096(1)	14(1)
C(8)	3886(1)	130(2)	3888(1)	14(1)
C(9)	5430(1)	-508(2)	3922(1)	18(1)
C(10)	3993(1)	5683(2)	3712(1)	23(1)
P(1)	2520(1)	1290(1)	2452(1)	10(1)
C(11)	1630(1)	1201(2)	2798(1)	13(1)
C(12)	1229(1)	2439(2)	2911(1)	16(1)
C(13)	525(1)	2369(2)	3147(1)	19(1)
C(14)	238(1)	1073(2)	3296(1)	21(1)
C(15)	669(1)	-148(2)	3231(1)	20(1)
C(16)	1359(1)	-84(2)	2979(1)	16(1)
C(17)	2012(1)	2260(2)	1583(1)	13(1)
C(18)	2510(1)	2348(2)	1147(1)	16(1)
C(19)	2159(1)	3026(2)	475(1)	18(1)
C(20)	1301(1)	3614(2)	227(1)	21(1)
C(21)	797(1)	3502(2)	644(1)	21(1)
C(22)	1146(1)	2824(2)	1319(1)	17(1)
C(23)	2454(1)	-471(2)	2049(1)	12(1)
C(24)	3179(1)	-1389(2)	2214(1)	14(1)
C(25)	3068(1)	-2703(2)	1880(1)	16(1)

C(26)	2233(1)	-3115(2)	1370(1)	18(1)
C(27)	1507(1)	-2191(2)	1190(1)	18(1)
C(28)	1616(1)	-890(2)	1525(1)	16(1)
C(1S)	1705(1)	5320(3)	4455(1)	42(1)
Cl(1S)	712(1)	5017(2)	4595(1)	30(1)
Cl(2S)	1469(1)	6198(1)	3587(1)	59(1)
Cl(3S)	674(4)	5419(8)	4500(6)	42(2)
Cl(4S)	1715(3)	6728(6)	3980(4)	86(2)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Ru(1)-C(1)	2.2012(15)
Ru(1)-C(8)	2.2436(15)
Ru(1)-C(6)	2.2666(14)
Ru(1)-C(2)	2.2823(15)
Ru(1)-C(3)	2.2838(14)
Ru(1)-C(7)	2.2845(14)
Ru(1)-Cl(2)	2.4193(3)
Ru(1)-Cl(1)	2.4206(4)
Ru(1)-P(1)	2.4231(4)
C(1)-C(2)	1.415(2)
C(1)-H(1A)	0.95(2)
C(1)-H(1B)	0.95(2)
C(2)-C(3)	1.400(2)
C(2)-C(10)	1.497(2)
C(3)-C(4)	1.509(2)
C(3)-H(3)	0.943(19)
C(4)-C(5)	1.528(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.515(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.411(2)
C(6)-H(6)	0.89(2)
C(7)-C(8)	1.4142(19)
C(7)-C(9)	1.500(2)
C(8)-H(8A)	0.977(19)
C(8)-H(8B)	0.95(2)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800

C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
P(1)-C(11)	1.8223(13)
P(1)-C(23)	1.8356(15)
P(1)-C(17)	1.8438(15)
C(11)-C(16)	1.388(2)
C(11)-C(12)	1.399(2)
C(12)-C(13)	1.391(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.385(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.381(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.3905(19)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(22)	1.3916(19)
C(17)-C(18)	1.3978(19)
C(18)-C(19)	1.389(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.389(2)
C(19)-H(19)	0.9500
C(20)-C(21)	1.377(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.395(2)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(24)	1.3894(19)
C(23)-C(28)	1.4038(18)
C(24)-C(25)	1.389(2)
C(24)-H(24)	0.9500
C(25)-C(26)	1.388(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.392(2)

C(26)-H(26)	0.9500
C(27)-C(28)	1.379(2)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(1S)-Cl(4S)	1.639(4)
C(1S)-Cl(3S)	1.703(5)
C(1S)-Cl(1S)	1.753(3)
C(1S)-Cl(2S)	1.821(3)
C(1S)-H(1S1)	0.9756
C(1S)-H(1S2)	0.9902
Cl(4S)-H(1S2)	1.7820

C(1)-Ru(1)-C(8)	162.29(5)
C(1)-Ru(1)-C(6)	132.02(6)
C(8)-Ru(1)-C(6)	64.34(5)
C(1)-Ru(1)-C(2)	36.75(5)
C(8)-Ru(1)-C(2)	155.48(5)
C(6)-Ru(1)-C(2)	95.76(6)
C(1)-Ru(1)-C(3)	64.22(5)
C(8)-Ru(1)-C(3)	133.38(5)
C(6)-Ru(1)-C(3)	70.13(5)
C(2)-Ru(1)-C(3)	35.72(5)
C(1)-Ru(1)-C(7)	160.81(5)
C(8)-Ru(1)-C(7)	36.38(5)
C(6)-Ru(1)-C(7)	36.11(6)
C(2)-Ru(1)-C(7)	130.14(5)
C(3)-Ru(1)-C(7)	98.14(5)
C(1)-Ru(1)-Cl(2)	85.27(4)
C(8)-Ru(1)-Cl(2)	98.64(4)
C(6)-Ru(1)-Cl(2)	101.69(4)
C(2)-Ru(1)-Cl(2)	99.45(4)
C(3)-Ru(1)-Cl(2)	80.80(4)
C(7)-Ru(1)-Cl(2)	84.38(4)
C(1)-Ru(1)-Cl(1)	93.08(4)

C(8)-Ru(1)-Cl(1)	81.81(4)
C(6)-Ru(1)-Cl(1)	82.24(4)
C(2)-Ru(1)-Cl(1)	81.34(4)
C(3)-Ru(1)-Cl(1)	101.92(4)
C(7)-Ru(1)-Cl(1)	98.25(4)
Cl(2)-Ru(1)-Cl(1)	175.857(12)
C(1)-Ru(1)-P(1)	81.62(4)
C(8)-Ru(1)-P(1)	81.57(4)
C(6)-Ru(1)-P(1)	145.85(4)
C(2)-Ru(1)-P(1)	116.51(4)
C(3)-Ru(1)-P(1)	143.67(4)
C(7)-Ru(1)-P(1)	113.35(4)
Cl(2)-Ru(1)-P(1)	84.593(12)
Cl(1)-Ru(1)-P(1)	91.413(13)
C(2)-C(1)-Ru(1)	74.75(9)
C(2)-C(1)-H(1A)	116.8(13)
Ru(1)-C(1)-H(1A)	120.3(13)
C(2)-C(1)-H(1B)	119.5(12)
Ru(1)-C(1)-H(1B)	100.9(12)
H(1A)-C(1)-H(1B)	116.5(17)
C(3)-C(2)-C(1)	115.78(14)
C(3)-C(2)-C(10)	123.29(14)
C(1)-C(2)-C(10)	120.86(14)
C(3)-C(2)-Ru(1)	72.20(9)
C(1)-C(2)-Ru(1)	68.51(9)
C(10)-C(2)-Ru(1)	126.74(11)
C(2)-C(3)-C(4)	125.25(14)
C(2)-C(3)-Ru(1)	72.08(8)
C(4)-C(3)-Ru(1)	119.28(10)
C(2)-C(3)-H(3)	118.8(11)
C(4)-C(3)-H(3)	113.4(11)
Ru(1)-C(3)-H(3)	95.1(12)
C(3)-C(4)-C(5)	105.46(13)
C(3)-C(4)-H(4A)	110.6

C(5)-C(4)-H(4A)	110.6
C(3)-C(4)-H(4B)	110.6
C(5)-C(4)-H(4B)	110.6
H(4A)-C(4)-H(4B)	108.8
C(6)-C(5)-C(4)	105.48(13)
C(6)-C(5)-H(5A)	110.6
C(4)-C(5)-H(5A)	110.6
C(6)-C(5)-H(5B)	110.6
C(4)-C(5)-H(5B)	110.6
H(5A)-C(5)-H(5B)	108.8
C(7)-C(6)-C(5)	124.97(14)
C(7)-C(6)-Ru(1)	72.64(8)
C(5)-C(6)-Ru(1)	118.54(10)
C(7)-C(6)-H(6)	117.2(13)
C(5)-C(6)-H(6)	115.3(13)
Ru(1)-C(6)-H(6)	94.3(13)
C(6)-C(7)-C(8)	116.46(13)
C(6)-C(7)-C(9)	122.43(13)
C(8)-C(7)-C(9)	120.99(14)
C(6)-C(7)-Ru(1)	71.25(8)
C(8)-C(7)-Ru(1)	70.23(8)
C(9)-C(7)-Ru(1)	125.34(10)
C(7)-C(8)-Ru(1)	73.38(9)
C(7)-C(8)-H(8A)	120.1(11)
Ru(1)-C(8)-H(8A)	98.9(12)
C(7)-C(8)-H(8B)	118.1(11)
Ru(1)-C(8)-H(8B)	120.4(12)
H(8A)-C(8)-H(8B)	116.4(15)
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5

C(2)-C(10)-H(10A)	109.5
C(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(11)-P(1)-C(23)	101.80(6)
C(11)-P(1)-C(17)	104.67(6)
C(23)-P(1)-C(17)	96.58(7)
C(11)-P(1)-Ru(1)	113.34(5)
C(23)-P(1)-Ru(1)	120.65(4)
C(17)-P(1)-Ru(1)	117.14(5)
C(16)-C(11)-C(12)	118.77(13)
C(16)-C(11)-P(1)	120.91(11)
C(12)-C(11)-P(1)	120.28(11)
C(13)-C(12)-C(11)	120.27(15)
C(13)-C(12)-H(12)	119.9
C(11)-C(12)-H(12)	119.9
C(14)-C(13)-C(12)	120.07(15)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(15)-C(14)-C(13)	119.95(13)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	120.09(16)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0
C(11)-C(16)-C(15)	120.65(15)
C(11)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(22)-C(17)-C(18)	118.58(13)
C(22)-C(17)-P(1)	123.79(11)
C(18)-C(17)-P(1)	117.50(10)
C(19)-C(18)-C(17)	120.68(13)

C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	120.12(14)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(21)-C(20)-C(19)	119.65(14)
C(21)-C(20)-H(20)	120.2
C(19)-C(20)-H(20)	120.2
C(20)-C(21)-C(22)	120.50(14)
C(20)-C(21)-H(21)	119.8
C(22)-C(21)-H(21)	119.8
C(17)-C(22)-C(21)	120.44(14)
C(17)-C(22)-H(22)	119.8
C(21)-C(22)-H(22)	119.8
C(24)-C(23)-C(28)	118.34(14)
C(24)-C(23)-P(1)	124.50(10)
C(28)-C(23)-P(1)	117.13(11)
C(25)-C(24)-C(23)	120.61(13)
C(25)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(26)-C(25)-C(24)	120.54(14)
C(26)-C(25)-H(25)	119.7
C(24)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	119.31(15)
C(25)-C(26)-H(26)	120.3
C(27)-C(26)-H(26)	120.3
C(28)-C(27)-C(26)	120.14(13)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(27)-C(28)-C(23)	121.05(13)
C(27)-C(28)-H(28)	119.5
C(23)-C(28)-H(28)	119.5
Cl(4S)-C(1S)-Cl(3S)	102.5(3)
Cl(4S)-C(1S)-Cl(1S)	116.2(2)

Cl(3S)-C(1S)-Cl(1S)	13.8(2)
Cl(4S)-C(1S)-Cl(2S)	29.0(3)
Cl(3S)-C(1S)-Cl(2S)	100.4(3)
Cl(1S)-C(1S)-Cl(2S)	111.21(13)
Cl(4S)-C(1S)-H(1S1)	125.9
Cl(3S)-C(1S)-H(1S1)	122.0
Cl(1S)-C(1S)-H(1S1)	109.3
Cl(2S)-C(1S)-H(1S1)	107.5
Cl(4S)-C(1S)-H(1S2)	81.3
Cl(3S)-C(1S)-H(1S2)	107.9
Cl(1S)-C(1S)-H(1S2)	110.4
Cl(2S)-C(1S)-H(1S2)	109.3
H(1S1)-C(1S)-H(1S2)	109.1
C(1S)-Cl(4S)-H(1S2)	33.3

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
Ru(1)	12(1)	9(1)	10(1)	0(1)	5(1)	-1(1)
Cl(1)	20(1)	17(1)	16(1)	-1(1)	11(1)	1(1)
Cl(2)	12(1)	13(1)	13(1)	-1(1)	6(1)	-1(1)
C(1)	20(1)	11(1)	14(1)	2(1)	7(1)	0(1)
C(2)	23(1)	10(1)	15(1)	1(1)	10(1)	-3(1)
C(3)	19(1)	14(1)	14(1)	-1(1)	8(1)	-7(1)
C(4)	23(1)	21(1)	16(1)	-2(1)	4(1)	-7(1)
C(5)	16(1)	25(1)	15(1)	-1(1)	3(1)	-5(1)
C(6)	16(1)	19(1)	11(1)	2(1)	5(1)	1(1)
C(7)	16(1)	15(1)	12(1)	5(1)	5(1)	2(1)
C(8)	16(1)	13(1)	15(1)	3(1)	7(1)	-1(1)
C(9)	17(1)	16(1)	19(1)	2(1)	6(1)	4(1)
C(10)	36(1)	13(1)	23(1)	-4(1)	14(1)	-3(1)
P(1)	11(1)	10(1)	12(1)	1(1)	5(1)	1(1)
C(11)	11(1)	15(1)	14(1)	0(1)	5(1)	1(1)
C(12)	17(1)	17(1)	16(1)	0(1)	8(1)	4(1)
C(13)	16(1)	27(1)	15(1)	-1(1)	7(1)	7(1)
C(14)	14(1)	34(1)	16(1)	-2(1)	8(1)	0(1)
C(15)	19(1)	24(1)	20(1)	-2(1)	11(1)	-5(1)
C(16)	17(1)	17(1)	18(1)	0(1)	9(1)	-2(1)
C(17)	13(1)	12(1)	13(1)	0(1)	5(1)	0(1)
C(18)	15(1)	19(1)	13(1)	-1(1)	5(1)	-1(1)
C(19)	22(1)	21(1)	13(1)	-1(1)	7(1)	-4(1)
C(20)	26(1)	19(1)	13(1)	1(1)	3(1)	0(1)
C(21)	18(1)	21(1)	18(1)	3(1)	3(1)	6(1)
C(22)	15(1)	19(1)	17(1)	1(1)	6(1)	4(1)
C(23)	13(1)	11(1)	14(1)	-1(1)	6(1)	0(1)
C(24)	14(1)	13(1)	16(1)	1(1)	7(1)	0(1)
C(25)	17(1)	11(1)	21(1)	0(1)	8(1)	1(1)

C(26)	22(1)	13(1)	21(1)	-4(1)	10(1)	-4(1)
C(27)	17(1)	17(1)	18(1)	-2(1)	4(1)	-4(1)
C(28)	13(1)	16(1)	17(1)	0(1)	4(1)	1(1)
C(1S)	21(1)	42(1)	61(2)	2(1)	13(1)	7(1)
Cl(1S)	21(1)	40(1)	27(1)	-9(1)	8(1)	3(1)
Cl(2S)	78(1)	32(1)	76(1)	21(1)	40(1)	18(1)
Cl(3S)	26(1)	51(4)	44(3)	-15(3)	6(1)	16(2)
Cl(4S)	33(2)	80(4)	136(5)	72(4)	25(2)	7(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(1A)	2949(13)	4430(20)	2481(11)	20(5)
H(1B)	3710(13)	3760(20)	2241(11)	17(5)
H(3)	5231(12)	3460(20)	3175(10)	13(4)
H(4A)	5574	4557	4595	25
H(4B)	6314	4428	4242	25
H(5A)	6312	1953	4309	24
H(5B)	6374	2482	5095	24
H(6)	4796(13)	2140(20)	4686(11)	16(5)
H(8A)	3563(12)	450(20)	4184(10)	14(4)
H(8B)	3664(12)	-700(20)	3609(10)	13(4)
H(9A)	5786	-1054	4358	26
H(9B)	5835	46	3765	26
H(9C)	5075	-1153	3531	26
H(10A)	4269	5459	4233	35
H(10B)	3338	5763	3559	35
H(10C)	4235	6580	3622	35
H(12)	1439	3332	2826	19
H(13)	242	3211	3207	23
H(14)	-256	1023	3442	25
H(15)	494	-1032	3359	24
H(16)	1648	-929	2930	19
H(18)	3094	1941	1311	19
H(19)	2505	3087	186	22
H(20)	1065	4091	-229	25
H(21)	206	3890	471	25
H(22)	790	2746	1601	21
H(24)	3756	-1116	2558	16
H(25)	3568	-3325	2002	19
H(26)	2158	-4017	1146	22

H(27)	935	-2456	835	22
H(28)	1115	-269	1399	19
H(1S1)	1990	4417	4443	51
H(1S2)	2129	5905	4855	51

Table S6. Torsion angles [°] for **1**.

C(8)-Ru(1)-C(1)-C(2)	143.60(17)
C(6)-Ru(1)-C(1)-C(2)	-11.24(12)
C(3)-Ru(1)-C(1)-C(2)	-30.66(8)
C(7)-Ru(1)-C(1)-C(2)	-55.2(2)
Cl(2)-Ru(1)-C(1)-C(2)	-112.72(8)
Cl(1)-Ru(1)-C(1)-C(2)	71.09(8)
P(1)-Ru(1)-C(1)-C(2)	162.06(8)
Ru(1)-C(1)-C(2)-C(3)	56.28(12)
Ru(1)-C(1)-C(2)-C(10)	-120.91(14)
C(1)-Ru(1)-C(2)-C(3)	-128.13(13)
C(8)-Ru(1)-C(2)-C(3)	77.65(15)
C(6)-Ru(1)-C(2)-C(3)	43.50(9)
C(7)-Ru(1)-C(2)-C(3)	31.20(11)
Cl(2)-Ru(1)-C(2)-C(3)	-59.39(8)
Cl(1)-Ru(1)-C(2)-C(3)	124.73(8)
P(1)-Ru(1)-C(2)-C(3)	-148.03(7)
C(8)-Ru(1)-C(2)-C(1)	-154.22(12)
C(6)-Ru(1)-C(2)-C(1)	171.63(9)
C(3)-Ru(1)-C(2)-C(1)	128.13(13)
C(7)-Ru(1)-C(2)-C(1)	159.33(8)
Cl(2)-Ru(1)-C(2)-C(1)	68.73(8)
Cl(1)-Ru(1)-C(2)-C(1)	-107.15(8)
P(1)-Ru(1)-C(2)-C(1)	-19.91(9)
C(1)-Ru(1)-C(2)-C(10)	113.21(17)
C(8)-Ru(1)-C(2)-C(10)	-41.0(2)
C(6)-Ru(1)-C(2)-C(10)	-75.16(14)
C(3)-Ru(1)-C(2)-C(10)	-118.66(17)
C(7)-Ru(1)-C(2)-C(10)	-87.46(15)
Cl(2)-Ru(1)-C(2)-C(10)	-178.06(13)
Cl(1)-Ru(1)-C(2)-C(10)	6.06(13)
P(1)-Ru(1)-C(2)-C(10)	93.30(13)
C(1)-C(2)-C(3)-C(4)	-168.02(14)

C(10)-C(2)-C(3)-C(4)	9.1(2)
Ru(1)-C(2)-C(3)-C(4)	-113.64(15)
C(1)-C(2)-C(3)-Ru(1)	-54.38(12)
C(10)-C(2)-C(3)-Ru(1)	122.74(15)
C(1)-Ru(1)-C(3)-C(2)	31.51(8)
C(8)-Ru(1)-C(3)-C(2)	-146.10(9)
C(6)-Ru(1)-C(3)-C(2)	-133.26(10)
C(7)-Ru(1)-C(3)-C(2)	-156.42(9)
Cl(2)-Ru(1)-C(3)-C(2)	120.67(8)
Cl(1)-Ru(1)-C(3)-C(2)	-56.14(8)
P(1)-Ru(1)-C(3)-C(2)	53.09(11)
C(1)-Ru(1)-C(3)-C(4)	152.45(14)
C(8)-Ru(1)-C(3)-C(4)	-25.16(16)
C(6)-Ru(1)-C(3)-C(4)	-12.32(12)
C(2)-Ru(1)-C(3)-C(4)	120.94(16)
C(7)-Ru(1)-C(3)-C(4)	-35.48(13)
Cl(2)-Ru(1)-C(3)-C(4)	-118.39(12)
Cl(1)-Ru(1)-C(3)-C(4)	64.80(12)
P(1)-Ru(1)-C(3)-C(4)	174.03(9)
C(2)-C(3)-C(4)-C(5)	125.88(16)
Ru(1)-C(3)-C(4)-C(5)	37.92(16)
C(3)-C(4)-C(5)-C(6)	-47.62(16)
C(4)-C(5)-C(6)-C(7)	130.89(15)
C(4)-C(5)-C(6)-Ru(1)	42.85(16)
C(1)-Ru(1)-C(6)-C(7)	-157.23(8)
C(8)-Ru(1)-C(6)-C(7)	31.02(8)
C(2)-Ru(1)-C(6)-C(7)	-163.96(8)
C(3)-Ru(1)-C(6)-C(7)	-138.66(9)
Cl(2)-Ru(1)-C(6)-C(7)	-63.04(8)
Cl(1)-Ru(1)-C(6)-C(7)	115.63(8)
P(1)-Ru(1)-C(6)-C(7)	34.63(12)
C(1)-Ru(1)-C(6)-C(5)	-36.33(15)
C(8)-Ru(1)-C(6)-C(5)	151.92(14)
C(2)-Ru(1)-C(6)-C(5)	-43.06(13)

C(3)-Ru(1)-C(6)-C(5)	-17.76(12)
C(7)-Ru(1)-C(6)-C(5)	120.90(16)
Cl(2)-Ru(1)-C(6)-C(5)	57.85(13)
Cl(1)-Ru(1)-C(6)-C(5)	-123.47(12)
P(1)-Ru(1)-C(6)-C(5)	155.53(9)
C(5)-C(6)-C(7)-C(8)	-168.49(14)
Ru(1)-C(6)-C(7)-C(8)	-55.40(11)
C(5)-C(6)-C(7)-C(9)	7.5(2)
Ru(1)-C(6)-C(7)-C(9)	120.54(13)
C(5)-C(6)-C(7)-Ru(1)	-113.09(14)
C(1)-Ru(1)-C(7)-C(6)	61.06(19)
C(8)-Ru(1)-C(7)-C(6)	-128.45(13)
C(2)-Ru(1)-C(7)-C(6)	21.08(11)
C(3)-Ru(1)-C(7)-C(6)	38.87(9)
Cl(2)-Ru(1)-C(7)-C(6)	118.71(8)
Cl(1)-Ru(1)-C(7)-C(6)	-64.52(8)
P(1)-Ru(1)-C(7)-C(6)	-159.67(7)
C(1)-Ru(1)-C(7)-C(8)	-170.48(15)
C(6)-Ru(1)-C(7)-C(8)	128.45(13)
C(2)-Ru(1)-C(7)-C(8)	149.53(9)
C(3)-Ru(1)-C(7)-C(8)	167.32(9)
Cl(2)-Ru(1)-C(7)-C(8)	-112.84(8)
Cl(1)-Ru(1)-C(7)-C(8)	63.94(9)
P(1)-Ru(1)-C(7)-C(8)	-31.21(9)
C(1)-Ru(1)-C(7)-C(9)	-55.9(2)
C(8)-Ru(1)-C(7)-C(9)	114.57(16)
C(6)-Ru(1)-C(7)-C(9)	-116.97(16)
C(2)-Ru(1)-C(7)-C(9)	-95.90(13)
C(3)-Ru(1)-C(7)-C(9)	-78.11(13)
Cl(2)-Ru(1)-C(7)-C(9)	1.73(12)
Cl(1)-Ru(1)-C(7)-C(9)	178.51(12)
P(1)-Ru(1)-C(7)-C(9)	83.36(12)
C(6)-C(7)-C(8)-Ru(1)	55.93(11)
C(9)-C(7)-C(8)-Ru(1)	-120.08(13)

C(1)-Ru(1)-C(8)-C(7)	169.71(16)
C(6)-Ru(1)-C(8)-C(7)	-30.80(8)
C(2)-Ru(1)-C(8)-C(7)	-69.09(15)
C(3)-Ru(1)-C(8)-C(7)	-17.39(12)
Cl(2)-Ru(1)-C(8)-C(7)	68.08(8)
Cl(1)-Ru(1)-C(8)-C(7)	-116.08(8)
P(1)-Ru(1)-C(8)-C(7)	151.25(9)
C(1)-Ru(1)-P(1)-C(11)	-107.14(7)
C(8)-Ru(1)-P(1)-C(11)	67.27(7)
C(6)-Ru(1)-P(1)-C(11)	63.98(9)
C(2)-Ru(1)-P(1)-C(11)	-95.26(7)
C(3)-Ru(1)-P(1)-C(11)	-126.70(9)
C(7)-Ru(1)-P(1)-C(11)	85.38(7)
Cl(2)-Ru(1)-P(1)-C(11)	166.86(6)
Cl(1)-Ru(1)-P(1)-C(11)	-14.24(6)
C(1)-Ru(1)-P(1)-C(23)	131.89(7)
C(8)-Ru(1)-P(1)-C(23)	-53.69(7)
C(6)-Ru(1)-P(1)-C(23)	-56.98(9)
C(2)-Ru(1)-P(1)-C(23)	143.78(7)
C(3)-Ru(1)-P(1)-C(23)	112.33(9)
C(7)-Ru(1)-P(1)-C(23)	-35.59(7)
Cl(2)-Ru(1)-P(1)-C(23)	45.90(5)
Cl(1)-Ru(1)-P(1)-C(23)	-135.20(5)
C(1)-Ru(1)-P(1)-C(17)	14.93(6)
C(8)-Ru(1)-P(1)-C(17)	-170.65(6)
C(6)-Ru(1)-P(1)-C(17)	-173.94(8)
C(2)-Ru(1)-P(1)-C(17)	26.82(7)
C(3)-Ru(1)-P(1)-C(17)	-4.63(9)
C(7)-Ru(1)-P(1)-C(17)	-152.55(6)
Cl(2)-Ru(1)-P(1)-C(17)	-71.06(5)
Cl(1)-Ru(1)-P(1)-C(17)	107.84(5)
C(23)-P(1)-C(11)-C(16)	25.34(13)
C(17)-P(1)-C(11)-C(16)	125.46(12)
Ru(1)-P(1)-C(11)-C(16)	-105.76(11)

C(23)-P(1)-C(11)-C(12)	-156.90(11)
C(17)-P(1)-C(11)-C(12)	-56.78(13)
Ru(1)-P(1)-C(11)-C(12)	72.00(12)
C(16)-C(11)-C(12)-C(13)	-4.8(2)
P(1)-C(11)-C(12)-C(13)	177.38(11)
C(11)-C(12)-C(13)-C(14)	2.2(2)
C(12)-C(13)-C(14)-C(15)	2.0(2)
C(13)-C(14)-C(15)-C(16)	-3.5(2)
C(12)-C(11)-C(16)-C(15)	3.3(2)
P(1)-C(11)-C(16)-C(15)	-178.86(11)
C(14)-C(15)-C(16)-C(11)	0.8(2)
C(11)-P(1)-C(17)-C(22)	3.01(15)
C(23)-P(1)-C(17)-C(22)	107.07(14)
Ru(1)-P(1)-C(17)-C(22)	-123.46(12)
C(11)-P(1)-C(17)-C(18)	-172.66(12)
C(23)-P(1)-C(17)-C(18)	-68.60(12)
Ru(1)-P(1)-C(17)-C(18)	60.87(13)
C(22)-C(17)-C(18)-C(19)	2.1(2)
P(1)-C(17)-C(18)-C(19)	178.04(12)
C(17)-C(18)-C(19)-C(20)	-0.6(2)
C(18)-C(19)-C(20)-C(21)	-1.1(3)
C(19)-C(20)-C(21)-C(22)	1.1(3)
C(18)-C(17)-C(22)-C(21)	-2.1(2)
P(1)-C(17)-C(22)-C(21)	-177.73(13)
C(20)-C(21)-C(22)-C(17)	0.5(3)
C(11)-P(1)-C(23)-C(24)	-126.56(12)
C(17)-P(1)-C(23)-C(24)	126.91(13)
Ru(1)-P(1)-C(23)-C(24)	-0.11(14)
C(11)-P(1)-C(23)-C(28)	55.31(12)
C(17)-P(1)-C(23)-C(28)	-51.22(12)
Ru(1)-P(1)-C(23)-C(28)	-178.23(9)
C(28)-C(23)-C(24)-C(25)	-1.6(2)
P(1)-C(23)-C(24)-C(25)	-179.74(11)
C(23)-C(24)-C(25)-C(26)	0.8(2)

C(24)-C(25)-C(26)-C(27)	0.6(2)
C(25)-C(26)-C(27)-C(28)	-1.1(2)
C(26)-C(27)-C(28)-C(23)	0.2(2)
C(24)-C(23)-C(28)-C(27)	1.2(2)
P(1)-C(23)-C(28)-C(27)	179.42(12)

Table S7. Crystal data and structure refinement for [{Ru(η^3: η^3-$C_{10}H_{16}$)Cl_2(PCy_3)]•CH_2Cl_2 (**2**).

Empirical formula	C_{29} H_{51} Cl_4 P Ru	
Formula weight	673.54	
Temperature	100(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Monoclinic, P 21/c	
Unit cell dimensions	a = 11.9906(3)Å	α = 90°.
	b = 10.1901(3)Å	β= 97.2730(10)°.
	c = 24.6438(7)Å	γ= 90°.
Volume	2986.89(14) A^3	
Z, Calculated density	4, 1.498 Mg/m^3	
Absorption coefficient	0.954 mm^{-1}	
F(000)	1408	
Crystal size	0.54 x 0.28 x 0.24 mm	
Theta range for data collection	1.71 to 30.69 °.	
Limiting indices	-17<=h<=17, -6<=k<=14, -34<=l<=35	
Reflections collected / unique	33891 / 9243 [R(int) = 0.0268]	
Completeness to theta = 30.69	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8033 and 0.6267	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9243 / 12 / 342	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1281	
R indices (all data)	R1 = 0.0545, wR2 = 0.1331	
Largest diff. peak and hole	2.382 and -2.577 $e.A^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	4452(1)	7334(1)	1272(1)	8(1)
Cl(1)	4116(1)	9489(1)	882(1)	13(1)
Cl(2)	4808(1)	5182(1)	1680(1)	13(1)
C(1)	5226(2)	6421(3)	581(1)	13(1)
C(2)	5963(2)	7424(3)	794(1)	12(1)
C(3)	6368(2)	7329(3)	1354(1)	13(1)
C(4)	6998(3)	8374(3)	1699(1)	15(1)
C(5)	6419(3)	8407(3)	2212(1)	15(1)
C(6)	5193(3)	8580(3)	1998(1)	13(1)
C(7)	4303(3)	7861(3)	2169(1)	13(1)
C(8)	3257(3)	7966(3)	1841(1)	14(1)
C(9)	4455(3)	6962(3)	2651(1)	17(1)
C(10)	6236(3)	8546(3)	444(1)	15(1)
P(1)	2653(1)	6635(1)	708(1)	9(1)
C(11)	2692(2)	6618(3)	-46(1)	11(1)
C(12)	1617(3)	6167(3)	-404(1)	15(1)
C(13)	1863(3)	5902(3)	-985(1)	18(1)
C(14)	2347(3)	7105(4)	-1238(1)	20(1)
C(15)	3384(3)	7606(3)	-874(1)	17(1)
C(16)	3119(3)	7873(3)	-295(1)	14(1)
C(17)	1354(2)	7561(3)	833(1)	12(1)
C(18)	212(3)	6882(3)	679(1)	15(1)
C(19)	-702(3)	7638(3)	928(2)	17(1)
C(20)	-777(3)	9054(3)	733(1)	17(1)
C(21)	366(3)	9731(3)	840(2)	18(1)
C(22)	1274(2)	8959(3)	599(1)	15(1)
C(23)	2202(2)	4928(3)	824(1)	11(1)
C(24)	1985(3)	4730(3)	1420(1)	13(1)
C(25)	1576(3)	3338(3)	1516(1)	16(1)

C(26)	2394(3)	2323(3)	1345(1)	16(1)
C(27)	2542(3)	2502(3)	747(1)	15(1)
C(28)	2982(3)	3872(3)	636(1)	12(1)
C(1S)	9769(8)	4841(11)	2477(4)	105(3)
Cl(1S)	10643(3)	6273(5)	2619(1)	160(2)
Cl(2S)	8395(2)	5327(2)	2443(1)	81(1)

Table S9. Bond lengths [Å] and angles [°] for **2**.

Ru(1)-C(8)	2.223(3)
Ru(1)-C(1)	2.241(3)
Ru(1)-C(3)	2.281(3)
Ru(1)-C(6)	2.281(3)
Ru(1)-C(2)	2.283(3)
Ru(1)-C(7)	2.304(3)
Ru(1)-Cl(1)	2.4104(7)
Ru(1)-Cl(2)	2.4270(7)
Ru(1)-P(1)	2.5163(8)
C(1)-C(2)	1.409(4)
C(1)-H(1A)	0.94(4)
C(1)-H(1B)	1.04(4)
C(2)-C(3)	1.405(4)
C(2)-C(10)	1.494(4)
C(3)-C(4)	1.506(4)
C(3)-H(3)	0.99(4)
C(4)-C(5)	1.517(4)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.508(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.403(4)
C(6)-H(6)	0.87(4)
C(7)-C(8)	1.407(4)
C(7)-C(9)	1.494(4)
C(8)-H(8A)	1.02(4)
C(8)-H(8B)	0.95(4)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800

C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
P(1)-C(23)	1.855(3)
P(1)-C(11)	1.865(3)
P(1)-C(17)	1.880(3)
C(11)-C(16)	1.533(4)
C(11)-C(12)	1.536(4)
C(11)-H(11)	1.0000
C(12)-C(13)	1.523(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.523(5)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.525(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.526(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(22)	1.536(4)
C(17)-C(18)	1.539(4)
C(17)-H(17)	1.0000
C(18)-C(19)	1.529(4)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.521(4)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.527(4)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900

C(21)-C(22)	1.524(4)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(28)	1.535(4)
C(23)-C(24)	1.538(4)
C(23)-H(23)	1.0000
C(24)-C(25)	1.529(4)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.522(4)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.517(4)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.529(4)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(1S)-Cl(2S)	1.712(9)
C(1S)-Cl(1S)	1.805(12)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900

C(8)-Ru(1)-C(1)	163.96(11)
C(8)-Ru(1)-C(3)	131.86(11)
C(1)-Ru(1)-C(3)	63.70(11)
C(8)-Ru(1)-C(6)	64.02(11)
C(1)-Ru(1)-C(6)	132.02(11)
C(3)-Ru(1)-C(6)	69.14(11)
C(8)-Ru(1)-C(2)	158.43(11)

C(1)-Ru(1)-C(2)	36.27(11)
C(3)-Ru(1)-C(2)	35.86(11)
C(6)-Ru(1)-C(2)	97.24(11)
C(8)-Ru(1)-C(7)	36.16(11)
C(1)-Ru(1)-C(7)	156.27(11)
C(3)-Ru(1)-C(7)	96.63(11)
C(6)-Ru(1)-C(7)	35.62(11)
C(2)-Ru(1)-C(7)	130.39(11)
C(8)-Ru(1)-Cl(1)	84.21(8)
C(1)-Ru(1)-Cl(1)	98.02(8)
C(3)-Ru(1)-Cl(1)	98.79(8)
C(6)-Ru(1)-Cl(1)	80.47(8)
C(2)-Ru(1)-Cl(1)	82.03(8)
C(7)-Ru(1)-Cl(1)	98.09(8)
C(8)-Ru(1)-Cl(2)	95.41(8)
C(1)-Ru(1)-Cl(2)	82.61(8)
C(3)-Ru(1)-Cl(2)	80.73(8)
C(6)-Ru(1)-Cl(2)	98.49(8)
C(2)-Ru(1)-Cl(2)	98.05(8)
C(7)-Ru(1)-Cl(2)	81.06(8)
Cl(1)-Ru(1)-Cl(2)	178.96(3)
C(8)-Ru(1)-P(1)	81.63(8)
C(1)-Ru(1)-P(1)	82.62(8)
C(3)-Ru(1)-P(1)	146.28(8)
C(6)-Ru(1)-P(1)	144.32(8)
C(2)-Ru(1)-P(1)	114.05(8)
C(7)-Ru(1)-P(1)	115.50(8)
Cl(1)-Ru(1)-P(1)	87.09(2)
Cl(2)-Ru(1)-P(1)	93.82(2)
C(2)-C(1)-Ru(1)	73.52(17)
C(2)-C(1)-H(1A)	117(3)
Ru(1)-C(1)-H(1A)	93(3)
C(2)-C(1)-H(1B)	116(2)
Ru(1)-C(1)-H(1B)	126(2)

H(1A)-C(1)-H(1B)	121(3)
C(3)-C(2)-C(1)	116.0(3)
C(3)-C(2)-C(10)	123.1(3)
C(1)-C(2)-C(10)	120.8(3)
C(3)-C(2)-Ru(1)	71.96(17)
C(1)-C(2)-Ru(1)	70.21(17)
C(10)-C(2)-Ru(1)	125.1(2)
C(2)-C(3)-C(4)	126.3(3)
C(2)-C(3)-Ru(1)	72.18(17)
C(4)-C(3)-Ru(1)	118.4(2)
C(2)-C(3)-H(3)	118(2)
C(4)-C(3)-H(3)	112(2)
Ru(1)-C(3)-H(3)	98(2)
C(3)-C(4)-C(5)	103.7(2)
C(3)-C(4)-H(4A)	111.0
C(5)-C(4)-H(4A)	111.0
C(3)-C(4)-H(4B)	111.0
C(5)-C(4)-H(4B)	111.0
H(4A)-C(4)-H(4B)	109.0
C(6)-C(5)-C(4)	103.9(2)
C(6)-C(5)-H(5A)	111.0
C(4)-C(5)-H(5A)	111.0
C(6)-C(5)-H(5B)	111.0
C(4)-C(5)-H(5B)	111.0
H(5A)-C(5)-H(5B)	109.0
C(7)-C(6)-C(5)	125.4(3)
C(7)-C(6)-Ru(1)	73.09(17)
C(5)-C(6)-Ru(1)	118.3(2)
C(7)-C(6)-H(6)	120(3)
C(5)-C(6)-H(6)	113(3)
Ru(1)-C(6)-H(6)	93(3)
C(6)-C(7)-C(8)	116.4(3)
C(6)-C(7)-C(9)	122.6(3)
C(8)-C(7)-C(9)	120.9(3)

C(6)-C(7)-Ru(1)	71.29(17)
C(8)-C(7)-Ru(1)	68.80(17)
C(9)-C(7)-Ru(1)	127.2(2)
C(7)-C(8)-Ru(1)	75.05(17)
C(7)-C(8)-H(8A)	116(2)
Ru(1)-C(8)-H(8A)	120(2)
C(7)-C(8)-H(8B)	112(3)
Ru(1)-C(8)-H(8B)	100(3)
H(8A)-C(8)-H(8B)	123(3)
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(2)-C(10)-H(10A)	109.5
C(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(23)-P(1)-C(11)	100.89(13)
C(23)-P(1)-C(17)	100.48(13)
C(11)-P(1)-C(17)	107.11(13)
C(23)-P(1)-Ru(1)	115.27(10)
C(11)-P(1)-Ru(1)	115.17(9)
C(17)-P(1)-Ru(1)	115.92(10)
C(16)-C(11)-C(12)	108.6(2)
C(16)-C(11)-P(1)	116.2(2)
C(12)-C(11)-P(1)	116.7(2)
C(16)-C(11)-H(11)	104.6
C(12)-C(11)-H(11)	104.6
P(1)-C(11)-H(11)	104.6
C(13)-C(12)-C(11)	110.1(3)

C(13)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.2
C(14)-C(13)-C(12)	111.8(3)
C(14)-C(13)-H(13A)	109.3
C(12)-C(13)-H(13A)	109.3
C(14)-C(13)-H(13B)	109.3
C(12)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	107.9
C(13)-C(14)-C(15)	110.7(3)
C(13)-C(14)-H(14A)	109.5
C(15)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
C(15)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	108.1
C(14)-C(15)-C(16)	111.0(3)
C(14)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15B)	109.4
C(16)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(15)-C(16)-C(11)	110.2(2)
C(15)-C(16)-H(16A)	109.6
C(11)-C(16)-H(16A)	109.6
C(15)-C(16)-H(16B)	109.6
C(11)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.1
C(22)-C(17)-C(18)	108.2(2)
C(22)-C(17)-P(1)	114.7(2)
C(18)-C(17)-P(1)	117.6(2)
C(22)-C(17)-H(17)	105.0
C(18)-C(17)-H(17)	105.0

P(1)-C(17)-H(17)	105.0
C(19)-C(18)-C(17)	109.6(3)
C(19)-C(18)-H(18A)	109.8
C(17)-C(18)-H(18A)	109.8
C(19)-C(18)-H(18B)	109.8
C(17)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.2
C(20)-C(19)-C(18)	111.6(3)
C(20)-C(19)-H(19A)	109.3
C(18)-C(19)-H(19A)	109.3
C(20)-C(19)-H(19B)	109.3
C(18)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	108.0
C(19)-C(20)-C(21)	111.0(3)
C(19)-C(20)-H(20A)	109.4
C(21)-C(20)-H(20A)	109.4
C(19)-C(20)-H(20B)	109.4
C(21)-C(20)-H(20B)	109.4
H(20A)-C(20)-H(20B)	108.0
C(22)-C(21)-C(20)	111.7(3)
C(22)-C(21)-H(21A)	109.3
C(20)-C(21)-H(21A)	109.3
C(22)-C(21)-H(21B)	109.3
C(20)-C(21)-H(21B)	109.3
H(21A)-C(21)-H(21B)	107.9
C(21)-C(22)-C(17)	110.2(3)
C(21)-C(22)-H(22A)	109.6
C(17)-C(22)-H(22A)	109.6
C(21)-C(22)-H(22B)	109.6
C(17)-C(22)-H(22B)	109.6
H(22A)-C(22)-H(22B)	108.1
C(28)-C(23)-C(24)	112.2(2)
C(28)-C(23)-P(1)	114.2(2)
C(24)-C(23)-P(1)	111.0(2)

C(28)-C(23)-H(23)	106.3
C(24)-C(23)-H(23)	106.3
P(1)-C(23)-H(23)	106.3
C(25)-C(24)-C(23)	111.5(2)
C(25)-C(24)-H(24A)	109.3
C(23)-C(24)-H(24A)	109.3
C(25)-C(24)-H(24B)	109.3
C(23)-C(24)-H(24B)	109.3
H(24A)-C(24)-H(24B)	108.0
C(26)-C(25)-C(24)	110.9(3)
C(26)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25A)	109.5
C(26)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	108.1
C(27)-C(26)-C(25)	110.3(3)
C(27)-C(26)-H(26A)	109.6
C(25)-C(26)-H(26A)	109.6
C(27)-C(26)-H(26B)	109.6
C(25)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	108.1
C(26)-C(27)-C(28)	111.6(2)
C(26)-C(27)-H(27A)	109.3
C(28)-C(27)-H(27A)	109.3
C(26)-C(27)-H(27B)	109.3
C(28)-C(27)-H(27B)	109.3
H(27A)-C(27)-H(27B)	108.0
C(27)-C(28)-C(23)	110.4(2)
C(27)-C(28)-H(28A)	109.6
C(23)-C(28)-H(28A)	109.6
C(27)-C(28)-H(28B)	109.6
C(23)-C(28)-H(28B)	109.6
H(28A)-C(28)-H(28B)	108.1
Cl(2S)-C(1S)-Cl(1S)	107.9(6)

Cl(2S)-C(1S)-H(1S1)	110.1
Cl(1S)-C(1S)-H(1S1)	110.1
Cl(2S)-C(1S)-H(1S2)	110.1
Cl(1S)-C(1S)-H(1S2)	110.1
H(1S1)-C(1S)-H(1S2)	108.4

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
Ru(1)	8(1)	8(1)	9(1)	0(1)	1(1)	1(1)
Cl(1)	12(1)	10(1)	15(1)	1(1)	1(1)	1(1)
Cl(2)	15(1)	11(1)	14(1)	2(1)	0(1)	1(1)
C(1)	12(1)	16(1)	12(1)	-3(1)	3(1)	2(1)
C(2)	10(1)	14(1)	13(1)	-1(1)	3(1)	1(1)
C(3)	9(1)	16(1)	13(1)	-1(1)	3(1)	1(1)
C(4)	11(1)	21(1)	14(1)	-2(1)	1(1)	-2(1)
C(5)	13(1)	19(1)	12(1)	-2(1)	-1(1)	-1(1)
C(6)	15(1)	12(1)	11(1)	-3(1)	1(1)	0(1)
C(7)	16(1)	13(1)	10(1)	-4(1)	3(1)	0(1)
C(8)	14(1)	16(1)	12(1)	-2(1)	4(1)	0(1)
C(9)	21(2)	19(1)	12(1)	1(1)	2(1)	-2(1)
C(10)	13(1)	18(1)	15(1)	1(1)	3(1)	-2(1)
P(1)	8(1)	8(1)	10(1)	1(1)	1(1)	0(1)
C(11)	12(1)	12(1)	10(1)	0(1)	1(1)	-1(1)
C(12)	14(1)	18(1)	12(1)	0(1)	0(1)	-3(1)
C(13)	19(2)	22(2)	13(1)	-2(1)	-1(1)	-4(1)
C(14)	27(2)	24(2)	11(1)	1(1)	1(1)	-4(1)
C(15)	23(2)	16(1)	13(1)	1(1)	5(1)	-4(1)
C(16)	17(1)	11(1)	13(1)	1(1)	2(1)	-2(1)
C(17)	9(1)	11(1)	15(1)	0(1)	2(1)	1(1)
C(18)	11(1)	12(1)	21(1)	0(1)	3(1)	-1(1)
C(19)	11(1)	16(1)	24(2)	3(1)	5(1)	1(1)
C(20)	10(1)	14(1)	26(2)	1(1)	2(1)	2(1)
C(21)	11(1)	15(1)	28(2)	-1(1)	3(1)	2(1)
C(22)	10(1)	11(1)	23(2)	2(1)	3(1)	2(1)
C(23)	11(1)	9(1)	13(1)	1(1)	2(1)	-1(1)
C(24)	16(1)	10(1)	13(1)	1(1)	4(1)	0(1)
C(25)	16(1)	13(1)	18(1)	4(1)	3(1)	-3(1)

C(26)	22(2)	11(1)	15(1)	1(1)	2(1)	-1(1)
C(27)	21(2)	9(1)	14(1)	-1(1)	1(1)	0(1)
C(28)	15(1)	10(1)	12(1)	1(1)	3(1)	1(1)
C(1S)	91(5)	143(6)	83(5)	-16(5)	18(4)	40(5)
Cl(1S)	107(2)	253(4)	126(2)	-119(3)	37(2)	-63(2)
Cl(2S)	80(1)	89(1)	76(1)	-23(1)	23(1)	-4(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(1A)	5310(30)	5600(40)	754(17)	12(9)
H(1B)	4910(30)	6490(40)	170(16)	11(9)
H(3)	6490(30)	6440(40)	1516(15)	7(9)
H(4A)	6939	9233	1510	18
H(4B)	7802	8141	1787	18
H(5A)	6544	7578	2420	18
H(5B)	6697	9149	2451	18
H(6)	5050(30)	9310(40)	1821(16)	8(9)
H(8A)	2640(40)	7340(40)	1933(17)	11(9)
H(8B)	3110(40)	8840(40)	1711(17)	15(10)
H(9A)	4500	7479	2989	26
H(9B)	5150	6458	2648	26
H(9C)	3815	6359	2634	26
H(10A)	6240	9364	653	23
H(10B)	5668	8602	121	23
H(10C)	6978	8407	327	23
H(11)	3265	5936	-104	14
H(12A)	1328	5358	-248	18
H(12B)	1032	6854	-408	18
H(13A)	2403	5167	-981	22
H(13B)	1159	5637	-1213	22
H(14A)	1771	7806	-1286	24
H(14B)	2553	6876	-1603	24
H(15A)	3652	8424	-1031	21
H(15B)	3992	6946	-862	21
H(16A)	2539	8567	-303	17
H(16B)	3804	8186	-65	17
H(17)	1424	7679	1239	14
H(18A)	29	6853	276	18

H(18B)	249	5969	818	18
H(19A)	-1436	7201	826	20
H(19B)	-535	7621	1332	20
H(20A)	-1328	9533	926	20
H(20B)	-1046	9077	336	20
H(21A)	310	10621	678	21
H(21B)	580	9826	1240	21
H(22A)	2007	9408	685	18
H(22B)	1092	8920	196	18
H(23)	1459	4812	594	13
H(24A)	2688	4899	1667	15
H(24B)	1413	5369	1509	15
H(25A)	1499	3222	1909	19
H(25B)	827	3204	1304	19
H(26A)	3131	2419	1573	19
H(26B)	2106	1430	1402	19
H(27A)	1810	2363	519	18
H(27B)	3075	1835	642	18
H(28A)	3028	3973	240	15
H(28B)	3748	3981	835	15
H(1S1)	9908	4442	2126	126
H(1S2)	9942	4182	2771	126

Table S12. Torsion angles [°] for **2**.

C(8)-Ru(1)-C(1)-C(2)	161.6(4)
C(3)-Ru(1)-C(1)-C(2)	-31.27(17)
C(6)-Ru(1)-C(1)-C(2)	-19.8(2)
C(7)-Ru(1)-C(1)-C(2)	-67.8(3)
Cl(1)-Ru(1)-C(1)-C(2)	64.61(17)
Cl(2)-Ru(1)-C(1)-C(2)	-114.55(17)
P(1)-Ru(1)-C(1)-C(2)	150.60(18)
Ru(1)-C(1)-C(2)-C(3)	57.2(2)
Ru(1)-C(1)-C(2)-C(10)	-119.8(3)
C(8)-Ru(1)-C(2)-C(3)	66.3(4)
C(1)-Ru(1)-C(2)-C(3)	-127.4(3)
C(6)-Ru(1)-C(2)-C(3)	37.94(19)
C(7)-Ru(1)-C(2)-C(3)	23.3(2)
Cl(1)-Ru(1)-C(2)-C(3)	117.20(17)
Cl(2)-Ru(1)-C(2)-C(3)	-61.75(17)
P(1)-Ru(1)-C(2)-C(3)	-159.61(15)
C(8)-Ru(1)-C(2)-C(1)	-166.3(3)
C(3)-Ru(1)-C(2)-C(1)	127.4(3)
C(6)-Ru(1)-C(2)-C(1)	165.34(18)
C(7)-Ru(1)-C(2)-C(1)	150.73(18)
Cl(1)-Ru(1)-C(2)-C(1)	-115.40(17)
Cl(2)-Ru(1)-C(2)-C(1)	65.65(17)
P(1)-Ru(1)-C(2)-C(1)	-32.22(19)
C(8)-Ru(1)-C(2)-C(10)	-51.9(4)
C(1)-Ru(1)-C(2)-C(10)	114.4(3)
C(3)-Ru(1)-C(2)-C(10)	-118.2(3)
C(6)-Ru(1)-C(2)-C(10)	-80.3(3)
C(7)-Ru(1)-C(2)-C(10)	-94.9(3)
Cl(1)-Ru(1)-C(2)-C(10)	-1.0(2)
Cl(2)-Ru(1)-C(2)-C(10)	-180.0(2)
P(1)-Ru(1)-C(2)-C(10)	82.1(3)
C(1)-C(2)-C(3)-C(4)	-168.9(3)

C(10)-C(2)-C(3)-C(4)	8.0(5)
Ru(1)-C(2)-C(3)-C(4)	-112.6(3)
C(1)-C(2)-C(3)-Ru(1)	-56.3(2)
C(10)-C(2)-C(3)-Ru(1)	120.6(3)
C(8)-Ru(1)-C(3)-C(2)	-153.13(17)
C(1)-Ru(1)-C(3)-C(2)	31.62(17)
C(6)-Ru(1)-C(3)-C(2)	-139.2(2)
C(7)-Ru(1)-C(3)-C(2)	-162.32(18)
Cl(1)-Ru(1)-C(3)-C(2)	-63.03(17)
Cl(2)-Ru(1)-C(3)-C(2)	117.91(17)
P(1)-Ru(1)-C(3)-C(2)	35.0(2)
C(8)-Ru(1)-C(3)-C(4)	-30.9(3)
C(1)-Ru(1)-C(3)-C(4)	153.8(3)
C(6)-Ru(1)-C(3)-C(4)	-17.0(2)
C(2)-Ru(1)-C(3)-C(4)	122.2(3)
C(7)-Ru(1)-C(3)-C(4)	-40.1(2)
Cl(1)-Ru(1)-C(3)-C(4)	59.2(2)
Cl(2)-Ru(1)-C(3)-C(4)	-119.9(2)
P(1)-Ru(1)-C(3)-C(4)	157.17(17)
C(2)-C(3)-C(4)-C(5)	133.3(3)
Ru(1)-C(3)-C(4)-C(5)	45.3(3)
C(3)-C(4)-C(5)-C(6)	-52.9(3)
C(4)-C(5)-C(6)-C(7)	133.6(3)
C(4)-C(5)-C(6)-Ru(1)	44.8(3)
C(8)-Ru(1)-C(6)-C(7)	30.47(17)
C(1)-Ru(1)-C(6)-C(7)	-149.11(18)
C(3)-Ru(1)-C(6)-C(7)	-138.1(2)
C(2)-Ru(1)-C(6)-C(7)	-160.74(18)
Cl(1)-Ru(1)-C(6)-C(7)	118.64(17)
Cl(2)-Ru(1)-C(6)-C(7)	-61.43(17)
P(1)-Ru(1)-C(6)-C(7)	47.4(2)
C(8)-Ru(1)-C(6)-C(5)	152.1(3)
C(1)-Ru(1)-C(6)-C(5)	-27.5(3)
C(3)-Ru(1)-C(6)-C(5)	-16.5(2)

C(2)-Ru(1)-C(6)-C(5)	-39.2(2)
C(7)-Ru(1)-C(6)-C(5)	121.6(3)
Cl(1)-Ru(1)-C(6)-C(5)	-119.8(2)
Cl(2)-Ru(1)-C(6)-C(5)	60.2(2)
P(1)-Ru(1)-C(6)-C(5)	169.03(16)
C(5)-C(6)-C(7)-C(8)	-166.6(3)
Ru(1)-C(6)-C(7)-C(8)	-53.5(2)
C(5)-C(6)-C(7)-C(9)	9.6(5)
Ru(1)-C(6)-C(7)-C(9)	122.7(3)
C(5)-C(6)-C(7)-Ru(1)	-113.1(3)
C(8)-Ru(1)-C(7)-C(6)	-129.4(3)
C(1)-Ru(1)-C(7)-C(6)	71.4(3)
C(3)-Ru(1)-C(7)-C(6)	38.95(19)
C(2)-Ru(1)-C(7)-C(6)	25.4(2)
Cl(1)-Ru(1)-C(7)-C(6)	-60.95(17)
Cl(2)-Ru(1)-C(7)-C(6)	118.44(17)
P(1)-Ru(1)-C(7)-C(6)	-151.58(15)
C(1)-Ru(1)-C(7)-C(8)	-159.2(3)
C(3)-Ru(1)-C(7)-C(8)	168.37(18)
C(6)-Ru(1)-C(7)-C(8)	129.4(3)
C(2)-Ru(1)-C(7)-C(8)	154.86(18)
Cl(1)-Ru(1)-C(7)-C(8)	68.47(18)
Cl(2)-Ru(1)-C(7)-C(8)	-112.14(18)
P(1)-Ru(1)-C(7)-C(8)	-22.16(19)
C(8)-Ru(1)-C(7)-C(9)	113.4(3)
C(1)-Ru(1)-C(7)-C(9)	-45.8(4)
C(3)-Ru(1)-C(7)-C(9)	-78.2(3)
C(6)-Ru(1)-C(7)-C(9)	-117.2(3)
C(2)-Ru(1)-C(7)-C(9)	-91.7(3)
Cl(1)-Ru(1)-C(7)-C(9)	-178.1(3)
Cl(2)-Ru(1)-C(7)-C(9)	1.3(3)
P(1)-Ru(1)-C(7)-C(9)	91.2(3)
C(6)-C(7)-C(8)-Ru(1)	54.8(2)
C(9)-C(7)-C(8)-Ru(1)	-121.5(3)

C(1)-Ru(1)-C(8)-C(7)	148.8(4)
C(3)-Ru(1)-C(8)-C(7)	-15.6(2)
C(6)-Ru(1)-C(8)-C(7)	-30.04(17)
C(2)-Ru(1)-C(8)-C(7)	-61.7(4)
Cl(1)-Ru(1)-C(8)-C(7)	-112.23(17)
Cl(2)-Ru(1)-C(8)-C(7)	66.79(17)
P(1)-Ru(1)-C(8)-C(7)	159.87(18)
C(8)-Ru(1)-P(1)-C(23)	-90.83(13)
C(1)-Ru(1)-P(1)-C(23)	86.11(13)
C(3)-Ru(1)-P(1)-C(23)	83.09(18)
C(6)-Ru(1)-P(1)-C(23)	-106.21(17)
C(2)-Ru(1)-P(1)-C(23)	104.65(13)
C(7)-Ru(1)-P(1)-C(23)	-77.83(13)
Cl(1)-Ru(1)-P(1)-C(23)	-175.41(11)
Cl(2)-Ru(1)-P(1)-C(23)	4.08(11)
C(8)-Ru(1)-P(1)-C(11)	152.25(13)
C(1)-Ru(1)-P(1)-C(11)	-30.81(13)
C(3)-Ru(1)-P(1)-C(11)	-33.84(18)
C(6)-Ru(1)-P(1)-C(11)	136.87(17)
C(2)-Ru(1)-P(1)-C(11)	-12.27(13)
C(7)-Ru(1)-P(1)-C(11)	165.25(13)
Cl(1)-Ru(1)-P(1)-C(11)	67.67(10)
Cl(2)-Ru(1)-P(1)-C(11)	-112.84(10)
C(8)-Ru(1)-P(1)-C(17)	26.11(13)
C(1)-Ru(1)-P(1)-C(17)	-156.95(13)
C(3)-Ru(1)-P(1)-C(17)	-159.97(17)
C(6)-Ru(1)-P(1)-C(17)	10.73(18)
C(2)-Ru(1)-P(1)-C(17)	-138.41(13)
C(7)-Ru(1)-P(1)-C(17)	39.11(14)
Cl(1)-Ru(1)-P(1)-C(17)	-58.46(11)
Cl(2)-Ru(1)-P(1)-C(17)	121.02(11)
C(23)-P(1)-C(11)-C(16)	-175.9(2)
C(17)-P(1)-C(11)-C(16)	79.4(2)
Ru(1)-P(1)-C(11)-C(16)	-51.1(2)

C(23)-P(1)-C(11)-C(12)	53.9(2)
C(17)-P(1)-C(11)-C(12)	-50.8(2)
Ru(1)-P(1)-C(11)-C(12)	178.67(18)
C(16)-C(11)-C(12)-C(13)	59.5(3)
P(1)-C(11)-C(12)-C(13)	-166.8(2)
C(11)-C(12)-C(13)-C(14)	-57.4(4)
C(12)-C(13)-C(14)-C(15)	54.6(4)
C(13)-C(14)-C(15)-C(16)	-54.9(4)
C(14)-C(15)-C(16)-C(11)	58.6(3)
C(12)-C(11)-C(16)-C(15)	-60.3(3)
P(1)-C(11)-C(16)-C(15)	165.7(2)
C(23)-P(1)-C(17)-C(22)	-161.3(2)
C(11)-P(1)-C(17)-C(22)	-56.3(2)
Ru(1)-P(1)-C(17)-C(22)	73.8(2)
C(23)-P(1)-C(17)-C(18)	-32.3(3)
C(11)-P(1)-C(17)-C(18)	72.6(2)
Ru(1)-P(1)-C(17)-C(18)	-157.25(19)
C(22)-C(17)-C(18)-C(19)	-60.9(3)
P(1)-C(17)-C(18)-C(19)	167.1(2)
C(17)-C(18)-C(19)-C(20)	58.5(4)
C(18)-C(19)-C(20)-C(21)	-54.2(4)
C(19)-C(20)-C(21)-C(22)	53.5(4)
C(20)-C(21)-C(22)-C(17)	-57.5(4)
C(18)-C(17)-C(22)-C(21)	60.6(3)
P(1)-C(17)-C(22)-C(21)	-165.9(2)
C(11)-P(1)-C(23)-C(28)	57.8(2)
C(17)-P(1)-C(23)-C(28)	167.7(2)
Ru(1)-P(1)-C(23)-C(28)	-66.9(2)
C(11)-P(1)-C(23)-C(24)	-174.1(2)
C(17)-P(1)-C(23)-C(24)	-64.2(2)
Ru(1)-P(1)-C(23)-C(24)	61.2(2)
C(28)-C(23)-C(24)-C(25)	-52.7(3)
P(1)-C(23)-C(24)-C(25)	178.2(2)
C(23)-C(24)-C(25)-C(26)	54.9(3)

C(24)-C(25)-C(26)-C(27)	-58.0(3)
C(25)-C(26)-C(27)-C(28)	59.0(3)
C(26)-C(27)-C(28)-C(23)	-56.1(3)
C(24)-C(23)-C(28)-C(27)	52.7(3)
P(1)-C(23)-C(28)-C(27)	-179.9(2)