Reactivity study of low-coordinate phosphaalkene IMes=PPh with Grubbs first-generation ruthenium benzylidene complexes

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Supporting Information

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Experimental

General Considerations. All manipulations involving air-sensitive materials were carried out in oven-dried glassware and performed under nitrogen using standard Schlenk line techniques or in a nitrogen atmosphere glovebox. All glassware and cannulae were dried overnight at 160 °C for at least 12 h prior to use. Solvents used in the preparation of air and/or moisture sensitive compounds were dried using an MBraun Solvent Purification System fitted with alumina columns and stored over molecular sieves under dinitrogen. IMes=P (**1**),[1a] $RuCl_2(PCy_3)_2(CHPh)$[1b] and $RuCl_2(PPh_3)_2(CHPh)$[1b] can be prepared using published procedures. Diallyl sulfide was purchased from Sigma-Aldrich and used without further purification. NMR solvents were purchased from Cambridge Isotope Laboratories and were degassed using three freeze-pump-thaw cycles. $CDCl_3$ was vacuum distilled from CaH_2 and stored under dinitrogen. NMR spectra were recorded on a Bruker AV 400 (^{1}H at 400 MHz, ^{13}C at 100MHz) or Bruker AV 300 (^{1}H at 300 MHz, ^{13}C at 75.5 MHz) spectrometer and are at room temperature unless otherwise stated. The spectra were referenced internally relative to the residual protio-solvent (^{1}H) and solvent (^{13}C) resonances and chemical shifts were reported with respect to δ = 0 ppm for tetramethylsilane. *J*-coupling constants are reported in Hertz (Hz). The multiplicity of signals is reported as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), broad (br) or a combination of any of these. Where ^{13}C spectra are reported, the ^{1}H and ^{13}C assignments were confirmed by two-dimensional ^{1}H-^{1}H, and ^{13}C-^{1}H correlation NMR experiments. The proton or carbon attributed to the resonance is sometimes italicized for clarity. Elemental composition was determined by Guelph Chemical Laboratories Incorporated.

Reaction of $RuCl_2(PPh_3)_2(CHPh)$ with IMes=PPh. A toluene solution of IMes=PPh (**1**) (30.1 mg, 73.0 μmol) was added slowly over 1 min to a toluene solution (5 mL) of

$RuCl_2(PPh_3)_2(CHPh)$ (52.1 mg, 66.2 μmol). The solution was stirred for 1 h at room temperature, in a color change from purple to yellowish brown and the formation of a light brown precipitate. The solution was filtered and dried under reduced pressure. Recrystallization by slow liquid diffusion of pentane into a saturated dichloromethane solution at –35 °C to afford $RuCl_2(IMes{=}PPh)(PPh_3)(CHPh)$ (**2**) as dark brown crystals (37.4 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 15.48 (dd, $^3J_{PH}$ = 9.2, 8.7 Hz, 1H, C*H*Ph), 8.14 (d, *J* = 7.4 Hz, 1H), 7.62–7.44 (m, 5H), 7.08–6.65 (m, 18H), 6.56 (t, *J* = 9.2, 2H), 6.47 (br s, 2H), 6.19 (br s, 1H), 5.97 (br s, 1H), 2.54 (br s, 3H), 2.29 (br s, 3H), 2.24 (br s, 3H), 2.10 (br s, 3H), 1.60 (br s, 6H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 299.7 (*C*HPh), 169.6, 168.3, 150.9, 141.2, 21.1–20.5, 19.4–19.0, 18.5, 17.9. ^{31}P{^{1}H} (121 MHz, $CDCl_3$): δ 64.8 (s, IMes=*P*Ph), 37.4 (s, *P*Ph_3). Anal. Calcd. for $C_{52}H_{50}Cl_2N_2P_2Ru$ (%): C, 66.66; H, 5.38; N, 2.99. Found (%): C, 66.46; H, 5.60; N, 2.92.

Reaction of $RuCl_2(PCy_3)_2(CHPh)$ with IMes=PPh. A toluene solution of IMes=PPh (**1**) (67.1 mg, 158 μmol) was added slowly over 1 min to a toluene solution (5 mL) of $RuCl_2(PCy_3)_2(CHPh)$ (92.7 mg, 113 μmol). The solution was stirred for 12 h at room temperature, resulting in a color change from purple to brown and the formation of a light brown precipitate. The volatiles were removed under reduced pressure. The product was recrystallized from pentane and dichloromethane to yield **3** as a light brown powder (85.7 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.00 (s, 1H), 8.11 (m, 2H), 7.66 (br s, 1H), 7.60 (s, 2H), 7.01 (s, 4H), 6.83 (br s, 2H), 2.57 (s, 3H), 2.18 (s, 12H), 1.76–0.90 (m, 30H). ^{31}P{^{1}H} (121 MHz, $CDCl_3$): δ 68.8 (d, *J* = 41.1 Hz), 64.2 (d, *J* = 41.1 Hz). Anal. Calcd. for $C_{52}H_{67}ClN_2P_2Ru$ (%): C, 67.99; H, 7.35; N, 3.05. Found (%): C, 68.28; H, 7.53; N, 2.77.

Ring-closing metathesis. The catalyst (0.006 mmol) was dissolved in $CDCl_3$ (0.5 mL). The solution was added to either an NMR tube fitted with a rubber septum or a scintillation vial fitted with a rubber septum. The neat substrate was added via syringe and the reaction stirred at either room temperature or at 70 °C. The reaction was monitored by ^{1}H NMR spectroscopy.

X-ray Crystallography. Crystallographic data were collected at the University of Toronto on a Bruker Kappa APEX-DUO diffractometer using a monochromated Mo-Kα radiation (Bruker Triumph; λ = 0.71073 Å) at 150K. Data were measured using a combination of ϕ scans and ω scans, and were processed using APEX2 and SAINT.[2] Absorption corrections were carried out using SADABS.[2] Both structures were solved using Superflip[3] and refined using WinGX[4] with SHELXS-97 for full-matrix least-squares refinement that was based on F^2.[5] All H atoms were included in calculated positions and allowed to refine in riding-motion approximation with U_{iso} tied to the carrier atom.

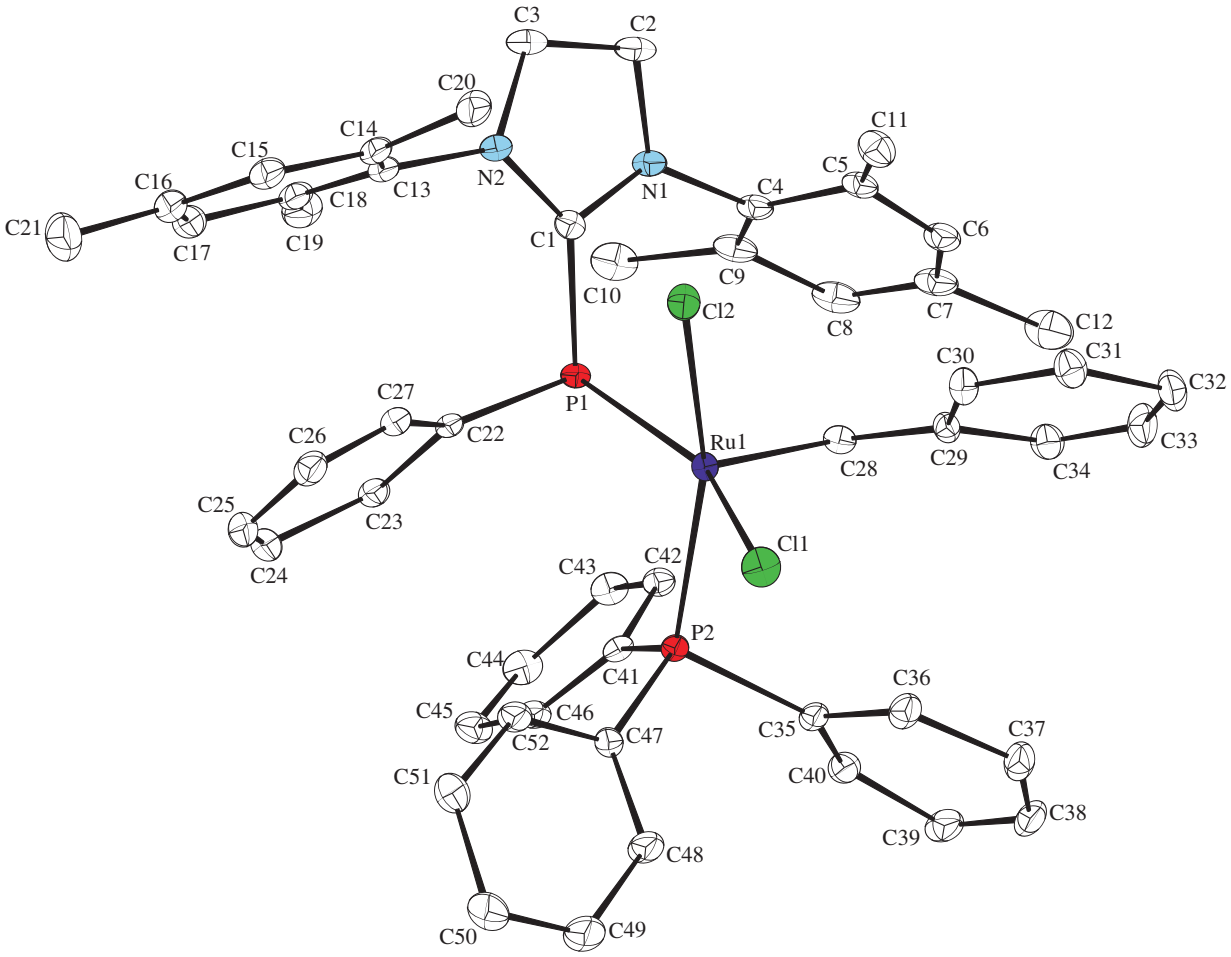

Figure S1. ORTEP diagram of complex **2** (30% probability level). All hydrogen atoms and one molecule of dichloromethane are omitted for clarity.

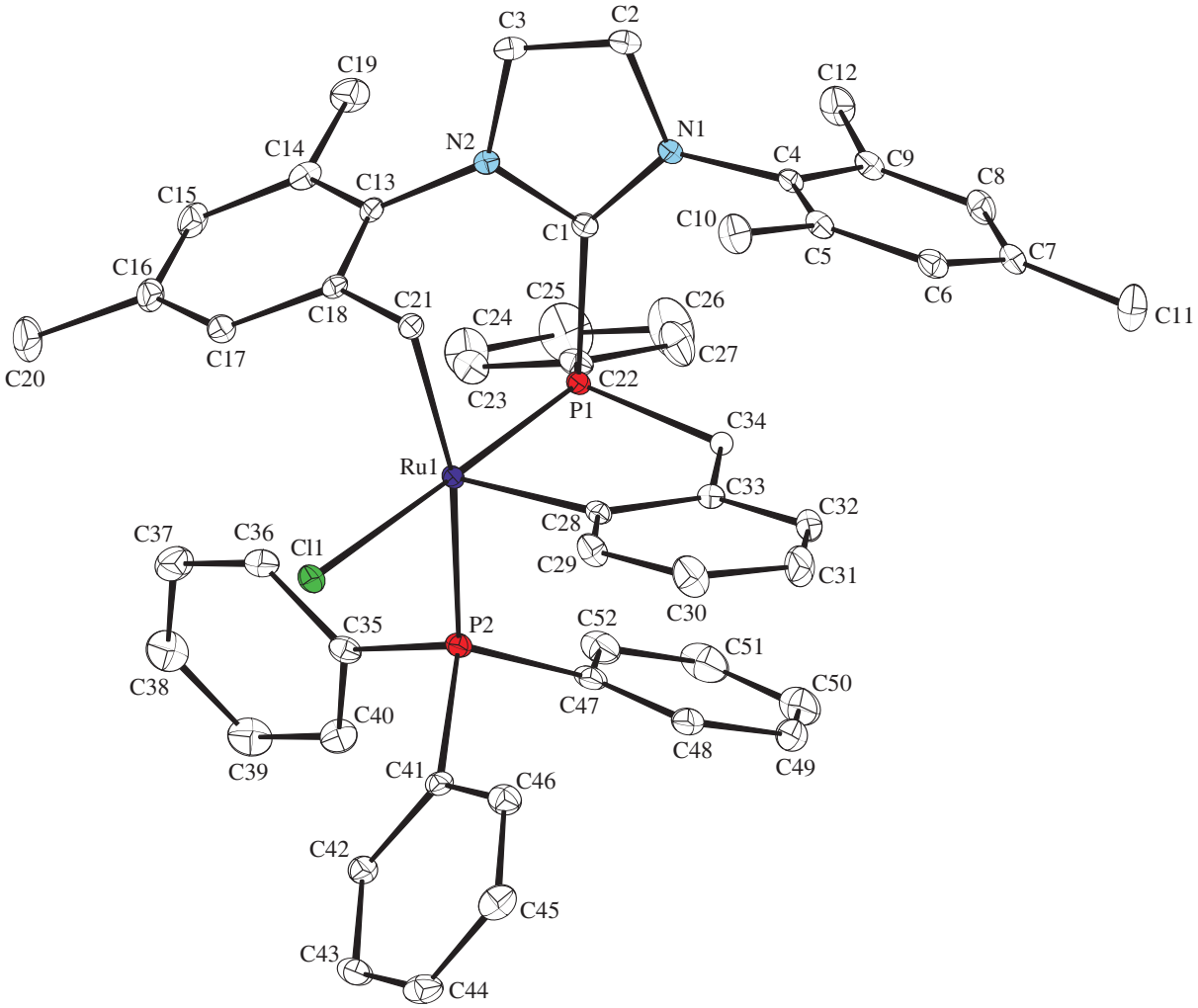

Figure S2. ORTEP diagram of complex **4** (30% probability level). All hydrogen atoms are omitted for clarity.

Table S1. Selected bond lengths and angles for **2** and **4.**

Bond lengths (Å)	**2**	**4**		**2**	**4**
Ru1–P1	2.3643(7)	2.1844(6)	P2–C35	1.840(3)	1.841(2)
Ru1–P2	2.3272(6)	2.3464(7)	P2–C41	1.824(2)	1.857(2)
Ru1–C28	1.841(3)	2.035(2)	P2–C47	1.827(2)	1.859(3)
Ru1–C21	–	2.157(2)	N1–C1	1.367(3)	1.352(3)
Ru–Cl1	2.3926(6)	2.4899(7)	N2–C1	1.361(3)	1.355(3)
Ru–Cl2	2.4012(6)	–	N2–C3	1.394(3)	1.384(3)
P1–C1	1.847(2)	1.883(2)	N1–C2	1.383(3)	1.391(3)
P1–C22	1.842(3)	1.842(2)	C2–C3	1.332(4)	1.346(3)
P1–C34	–	1.839(2)			
Bond Angles (deg)					
P1–Ru1–P2	90.61(2)	95.21(3)	P1–Ru1–C28	96.43(8)	80.51(6)
Cl1–Ru–Cl2	86.45(2)	–	Ru1–C28–C29	126.40(18)	–
P1–Ru1–Cl1	158.18(2)	177.83(2)	P2–Ru1–C21	–	92.48(6)
P2–Ru1–Cl2	168.06(2)	–	Ru1–C21–C18	–	89.8(1)

Table S2. Crystal data and structure refinement for compound **2**.

CCDC deposition number	845573	
Identification code	d1324	
Empirical formula	C53 H52 Cl4 N2 P2 Ru	
Formula weight	1021.78	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 39.366(4) Å	α= 90°.
	b = 10.3992(11) Å	β= 104.747(2)°.
	c = 24.505(3) Å	γ = 90°.
Volume	9701.5(18) $Å^3$	
Z	8	
Density (calculated)	1.399 Mg/m^3	
Absorption coefficient	0.648 mm^{-1}	
F(000)	4208	
Crystal size	0.36 x 0.22 x 0.20 mm^3	
Theta range for data collection	1.07 to 27.52°.	
Index ranges	-50<=h<=51, -13<=k<=13, -31<=l<=31	
Reflections collected	42646	
Independent reflections	11151 [R(int) = 0.0520]	
Completeness to theta = 27.52°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11151 / 0 / 569	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.0736	
R indices (all data)	R1 = 0.0579, wR2 = 0.0834	
Largest diff. peak and hole	0.589 and -0.555 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1800(1)	3994(2)	2471(1)	21(1)
C(1S)	949(1)	8740(4)	2356(2)	72(1)
C(2)	2373(1)	4551(3)	2768(1)	33(1)
C(3)	2272(1)	4136(3)	3217(1)	35(1)
C(4)	2083(1)	4926(2)	1755(1)	24(1)
C(5)	2240(1)	4158(2)	1423(1)	24(1)
C(6)	2241(1)	4616(3)	891(1)	28(1)
C(7)	2100(1)	5807(3)	694(1)	33(1)
C(8)	1951(1)	6547(3)	1046(1)	34(1)
C(9)	1943(1)	6144(2)	1583(1)	29(1)
C(10)	1792(1)	6998(2)	1957(1)	37(1)
C(11)	2411(1)	2894(3)	1629(1)	33(1)
C(12)	2124(1)	6269(3)	124(1)	47(1)
C(13)	1721(1)	3410(3)	3431(1)	25(1)
C(14)	1747(1)	2154(3)	3633(1)	27(1)
C(15)	1546(1)	1829(3)	4004(1)	31(1)
C(16)	1337(1)	2720(3)	4189(1)	35(1)
C(17)	1338(1)	3979(3)	4001(1)	34(1)
C(18)	1527(1)	4357(3)	3623(1)	28(1)
C(19)	1527(1)	5732(3)	3431(1)	37(1)
C(20)	1983(1)	1180(3)	3462(1)	35(1)
C(21)	1122(1)	2332(4)	4593(1)	52(1)
C(22)	1057(1)	3617(2)	2370(1)	19(1)
C(23)	803(1)	4549(3)	2381(1)	25(1)
C(24)	533(1)	4306(3)	2636(1)	34(1)
C(25)	513(1)	3134(3)	2891(1)	36(1)
C(26)	762(1)	2202(3)	2886(1)	31(1)
C(27)	1030(1)	2425(2)	2624(1)	23(1)
C(28)	1495(1)	2796(2)	832(1)	21(1)
C(29)	1699(1)	2039(2)	522(1)	21(1)
C(30)	1817(1)	782(2)	674(1)	27(1)
C(31)	2002(1)	122(3)	351(1)	31(1)
C(32)	2063(1)	663(3)	-128(1)	35(1)
C(33)	1943(1)	1884(3)	-290(1)	39(1)

C(34)	1764(1)	2565(3)	34(1)	29(1)
C(35)	735(1)	3142(2)	35(1)	22(1)
C(36)	849(1)	2083(3)	-219(1)	30(1)
C(37)	835(1)	2097(3)	-792(1)	36(1)
C(38)	707(1)	3159(3)	-1116(1)	39(1)
C(39)	592(1)	4214(3)	-872(1)	36(1)
C(40)	603(1)	4209(3)	-299(1)	27(1)
C(41)	664(1)	4779(2)	921(1)	18(1)
C(42)	918(1)	5698(2)	897(1)	22(1)
C(43)	855(1)	6993(2)	959(1)	27(1)
C(44)	539(1)	7384(2)	1055(1)	30(1)
C(45)	288(1)	6487(2)	1092(1)	30(1)
C(46)	349(1)	5182(2)	1022(1)	24(1)
C(47)	367(1)	2228(2)	836(1)	20(1)
C(48)	103(1)	1915(3)	364(1)	33(1)
C(49)	-182(1)	1186(3)	415(1)	45(1)
C(50)	-208(1)	779(3)	936(1)	40(1)
C(51)	50(1)	1108(3)	1415(1)	35(1)
C(52)	334(1)	1830(2)	1365(1)	27(1)
Cl(1)	1030(1)	149(1)	982(1)	31(1)
Cl(1S)	526(1)	8562(1)	2453(1)	78(1)
Cl(2)	1712(1)	961(1)	2006(1)	28(1)
Cl(2S)	1263(1)	8941(1)	2995(1)	65(1)
N(1)	2083(1)	4476(2)	2311(1)	23(1)
N(2)	1919(1)	3791(2)	3036(1)	25(1)
P(1)	1370(1)	4001(1)	1947(1)	18(1)
P(2)	761(1)	3106(1)	796(1)	17(1)
Ru(1)	1270(1)	2176(1)	1352(1)	17(1)

Table S4. Bond lengths [Å] and angles [°] for compound **2**.

C(1)-N(2)	1.361(3)
C(1)-N(1)	1.367(3)
C(1)-P(1)	1.847(2)
C(1S)-Cl(2S)	1.745(4)
C(1S)-Cl(1S)	1.751(4)
C(2)-C(3)	1.332(4)
C(2)-N(1)	1.383(3)
C(3)-N(2)	1.394(3)
C(4)-C(5)	1.394(4)
C(4)-C(9)	1.402(3)
C(4)-N(1)	1.439(3)
C(5)-C(6)	1.389(4)
C(5)-C(11)	1.503(3)
C(6)-C(7)	1.393(4)
C(7)-C(8)	1.390(4)
C(7)-C(12)	1.503(4)
C(8)-C(9)	1.390(4)
C(9)-C(10)	1.503(4)
C(13)-C(14)	1.391(4)
C(13)-C(18)	1.398(4)
C(13)-N(2)	1.445(3)
C(14)-C(15)	1.391(4)
C(14)-C(20)	1.504(4)
C(15)-C(16)	1.390(4)
C(16)-C(17)	1.389(4)
C(16)-C(21)	1.510(4)
C(17)-C(18)	1.386(4)
C(18)-C(19)	1.505(4)
C(22)-C(23)	1.398(3)
C(22)-C(27)	1.404(3)
C(22)-P(1)	1.843(3)
C(23)-C(24)	1.390(4)
C(24)-C(25)	1.380(4)
C(25)-C(26)	1.381(4)
C(26)-C(27)	1.387(4)
C(28)-C(29)	1.469(3)
C(28)-Ru(1)	1.841(3)

C(29)-C(34)	1.396(4)
C(29)-C(30)	1.406(3)
C(30)-C(31)	1.385(4)
C(31)-C(32)	1.378(4)
C(32)-C(33)	1.378(4)
C(33)-C(34)	1.383(4)
C(35)-C(36)	1.394(4)
C(35)-C(40)	1.398(4)
C(35)-P(2)	1.840(3)
C(36)-C(37)	1.389(4)
C(37)-C(38)	1.379(4)
C(38)-C(39)	1.381(4)
C(39)-C(40)	1.395(4)
C(41)-C(46)	1.389(3)
C(41)-C(42)	1.394(3)
C(41)-P(2)	1.824(2)
C(42)-C(43)	1.384(3)
C(43)-C(44)	1.384(4)
C(44)-C(45)	1.379(4)
C(45)-C(46)	1.397(3)
C(47)-C(48)	1.383(3)
C(47)-C(52)	1.396(4)
C(47)-P(2)	1.827(2)
C(48)-C(49)	1.385(4)
C(49)-C(50)	1.373(4)
C(50)-C(51)	1.384(4)
C(51)-C(52)	1.381(3)
Cl(1)-Ru(1)	2.3925(6)
Cl(2)-Ru(1)	2.4012(6)
P(1)-Ru(1)	2.3643(7)
P(2)-Ru(1)	2.3272(6)

N(2)-C(1)-N(1)	104.77(19)
N(2)-C(1)-P(1)	136.43(19)
N(1)-C(1)-P(1)	118.01(18)
Cl(2S)-C(1S)-Cl(1S)	111.8(2)
C(3)-C(2)-N(1)	107.0(2)
C(2)-C(3)-N(2)	107.7(2)
C(5)-C(4)-C(9)	122.7(3)

C(5)-C(4)-N(1)	118.2(2)
C(9)-C(4)-N(1)	119.0(2)
C(6)-C(5)-C(4)	117.4(2)
C(6)-C(5)-C(11)	120.5(2)
C(4)-C(5)-C(11)	122.1(2)
C(5)-C(6)-C(7)	122.2(3)
C(8)-C(7)-C(6)	118.1(3)
C(8)-C(7)-C(12)	122.4(3)
C(6)-C(7)-C(12)	119.5(3)
C(9)-C(8)-C(7)	122.4(3)
C(8)-C(9)-C(4)	117.1(3)
C(8)-C(9)-C(10)	120.5(2)
C(4)-C(9)-C(10)	122.5(3)
C(14)-C(13)-C(18)	122.6(3)
C(14)-C(13)-N(2)	119.5(2)
C(18)-C(13)-N(2)	117.8(2)
C(15)-C(14)-C(13)	117.3(2)
C(15)-C(14)-C(20)	120.8(3)
C(13)-C(14)-C(20)	121.9(2)
C(16)-C(15)-C(14)	122.3(3)
C(17)-C(16)-C(15)	117.9(3)
C(17)-C(16)-C(21)	121.3(3)
C(15)-C(16)-C(21)	120.8(3)
C(18)-C(17)-C(16)	122.5(3)
C(17)-C(18)-C(13)	117.2(3)
C(17)-C(18)-C(19)	121.3(3)
C(13)-C(18)-C(19)	121.5(3)
C(23)-C(22)-C(27)	117.9(2)
C(23)-C(22)-P(1)	116.32(19)
C(27)-C(22)-P(1)	125.37(18)
C(24)-C(23)-C(22)	121.1(3)
C(25)-C(24)-C(23)	120.2(3)
C(24)-C(25)-C(26)	119.6(3)
C(25)-C(26)-C(27)	120.8(3)
C(26)-C(27)-C(22)	120.4(2)
C(29)-C(28)-Ru(1)	126.40(18)
C(34)-C(29)-C(30)	118.1(2)
C(34)-C(29)-C(28)	118.5(2)
C(30)-C(29)-C(28)	123.3(2)

C(31)-C(30)-C(29)	119.8(3)
C(32)-C(31)-C(30)	121.0(3)
C(33)-C(32)-C(31)	120.0(3)
C(32)-C(33)-C(34)	119.7(3)
C(33)-C(34)-C(29)	121.5(3)
C(36)-C(35)-C(40)	118.6(2)
C(36)-C(35)-P(2)	119.7(2)
C(40)-C(35)-P(2)	121.6(2)
C(37)-C(36)-C(35)	120.6(3)
C(38)-C(37)-C(36)	120.3(3)
C(37)-C(38)-C(39)	120.0(3)
C(38)-C(39)-C(40)	120.2(3)
C(39)-C(40)-C(35)	120.3(3)
C(46)-C(41)-C(42)	118.8(2)
C(46)-C(41)-P(2)	123.56(18)
C(42)-C(41)-P(2)	117.60(18)
C(43)-C(42)-C(41)	120.8(2)
C(44)-C(43)-C(42)	119.8(2)
C(45)-C(44)-C(43)	120.1(2)
C(44)-C(45)-C(46)	120.1(2)
C(41)-C(46)-C(45)	120.3(2)
C(48)-C(47)-C(52)	118.7(2)
C(48)-C(47)-P(2)	122.7(2)
C(52)-C(47)-P(2)	118.54(18)
C(47)-C(48)-C(49)	120.4(3)
C(50)-C(49)-C(48)	120.3(3)
C(49)-C(50)-C(51)	120.1(3)
C(52)-C(51)-C(50)	119.6(3)
C(51)-C(52)-C(47)	120.8(2)
C(1)-N(1)-C(2)	110.6(2)
C(1)-N(1)-C(4)	125.82(19)
C(2)-N(1)-C(4)	123.5(2)
C(1)-N(2)-C(3)	109.9(2)
C(1)-N(2)-C(13)	128.3(2)
C(3)-N(2)-C(13)	121.5(2)
C(22)-P(1)-C(1)	103.53(11)
C(22)-P(1)-Ru(1)	98.20(8)
C(1)-P(1)-Ru(1)	113.81(8)
C(41)-P(2)-C(47)	104.46(11)

C(41)-P(2)-C(35)	101.00(11)
C(47)-P(2)-C(35)	103.68(11)
C(41)-P(2)-Ru(1)	118.95(7)
C(47)-P(2)-Ru(1)	112.19(8)
C(35)-P(2)-Ru(1)	114.79(8)
C(28)-Ru(1)-P(2)	86.69(7)
C(28)-Ru(1)-P(1)	96.43(8)
P(2)-Ru(1)-P(1)	90.61(2)
C(28)-Ru(1)-Cl(1)	105.05(8)
P(2)-Ru(1)-Cl(1)	86.89(2)
P(1)-Ru(1)-Cl(1)	158.18(2)
C(28)-Ru(1)-Cl(2)	104.61(7)
P(2)-Ru(1)-Cl(2)	168.06(2)
P(1)-Ru(1)-Cl(2)	91.89(2)
Cl(1)-Ru(1)-Cl(2)	86.45(2)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **2**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	20(1)	18(1)	25(2)	-1(1)	5(1)	1(1)
C(1S)	127(4)	52(2)	42(2)	-4(2)	34(2)	-25(2)
C(2)	17(1)	41(2)	34(2)	-2(1)	-4(1)	-2(1)
C(3)	20(1)	48(2)	31(2)	-1(2)	-5(1)	-1(1)
C(4)	16(1)	26(1)	27(2)	2(1)	1(1)	-7(1)
C(5)	15(1)	27(1)	30(2)	5(1)	3(1)	-7(1)
C(6)	18(1)	35(1)	31(2)	4(1)	4(1)	-7(1)
C(7)	19(1)	42(2)	35(2)	14(1)	0(1)	-9(1)
C(8)	23(1)	26(1)	48(2)	13(1)	1(1)	-6(1)
C(9)	18(1)	23(1)	42(2)	4(1)	0(1)	-8(1)
C(10)	35(1)	21(1)	52(2)	-4(1)	5(1)	-3(1)
C(11)	29(1)	31(1)	38(2)	6(1)	11(1)	5(1)
C(12)	36(2)	57(2)	48(2)	24(2)	8(2)	-4(2)
C(13)	20(1)	34(1)	18(1)	-2(1)	-1(1)	4(1)
C(14)	24(1)	38(2)	16(1)	-1(1)	-1(1)	6(1)
C(15)	30(1)	38(2)	22(2)	4(1)	1(1)	5(1)
C(16)	29(1)	51(2)	23(2)	0(1)	4(1)	7(1)
C(17)	27(1)	44(2)	29(2)	-8(1)	4(1)	10(1)
C(18)	25(1)	35(1)	19(2)	-3(1)	-2(1)	6(1)
C(19)	39(2)	32(2)	36(2)	-8(1)	3(1)	3(1)
C(20)	36(2)	44(2)	23(2)	7(1)	5(1)	15(1)
C(21)	50(2)	71(2)	43(2)	7(2)	24(2)	6(2)
C(22)	17(1)	22(1)	16(1)	-4(1)	1(1)	-2(1)
C(23)	23(1)	29(1)	21(2)	-6(1)	2(1)	0(1)
C(24)	23(1)	48(2)	30(2)	-8(1)	7(1)	5(1)
C(25)	27(1)	57(2)	26(2)	-6(2)	12(1)	-8(1)
C(26)	35(1)	37(2)	21(2)	1(1)	7(1)	-8(1)
C(27)	23(1)	26(1)	19(1)	-2(1)	2(1)	-1(1)
C(28)	19(1)	17(1)	25(2)	1(1)	4(1)	-1(1)
C(29)	20(1)	23(1)	23(1)	-3(1)	9(1)	-3(1)
C(30)	32(1)	26(1)	27(2)	-2(1)	13(1)	-1(1)
C(31)	33(1)	26(1)	36(2)	-4(1)	14(1)	1(1)
C(32)	33(1)	41(2)	38(2)	-12(1)	21(1)	-4(1)
C(33)	43(2)	50(2)	29(2)	1(2)	20(1)	-6(1)

C(34)	28(1)	32(1)	29(2)	4(1)	10(1)	-4(1)
C(35)	21(1)	27(1)	18(1)	-3(1)	5(1)	-11(1)
C(36)	33(1)	31(1)	25(2)	-6(1)	9(1)	-11(1)
C(37)	36(1)	45(2)	30(2)	-15(2)	15(1)	-17(1)
C(38)	37(2)	62(2)	18(2)	-6(2)	8(1)	-21(2)
C(39)	31(1)	51(2)	23(2)	8(1)	3(1)	-14(1)
C(40)	24(1)	34(1)	23(2)	2(1)	6(1)	-6(1)
C(41)	22(1)	16(1)	16(1)	1(1)	0(1)	-1(1)
C(42)	21(1)	21(1)	23(1)	0(1)	3(1)	-2(1)
C(43)	30(1)	20(1)	29(2)	1(1)	4(1)	-4(1)
C(44)	34(1)	19(1)	34(2)	-2(1)	2(1)	4(1)
C(45)	24(1)	28(1)	36(2)	-4(1)	4(1)	4(1)
C(46)	20(1)	25(1)	25(2)	-3(1)	2(1)	-3(1)
C(47)	20(1)	18(1)	23(1)	-3(1)	7(1)	-4(1)
C(48)	28(1)	47(2)	24(2)	-2(1)	5(1)	-16(1)
C(49)	33(2)	63(2)	37(2)	-14(2)	6(1)	-26(2)
C(50)	30(1)	43(2)	50(2)	-7(2)	14(1)	-21(1)
C(51)	34(1)	37(2)	37(2)	5(1)	16(1)	-8(1)
C(52)	23(1)	31(1)	26(2)	0(1)	5(1)	-9(1)
Cl(1)	38(1)	14(1)	41(1)	-4(1)	12(1)	-7(1)
Cl(1S)	102(1)	73(1)	56(1)	9(1)	15(1)	12(1)
Cl(2)	32(1)	26(1)	26(1)	6(1)	9(1)	10(1)
Cl(2S)	105(1)	43(1)	50(1)	7(1)	23(1)	-7(1)
N(1)	18(1)	25(1)	23(1)	1(1)	0(1)	-3(1)
N(2)	20(1)	33(1)	20(1)	1(1)	1(1)	2(1)
P(1)	16(1)	16(1)	20(1)	-1(1)	2(1)	0(1)
P(2)	18(1)	15(1)	18(1)	-2(1)	4(1)	-5(1)
Ru(1)	19(1)	13(1)	19(1)	0(1)	7(1)	-1(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound **2**.

	x	y	z	U(eq)
H(1S1)	1007	7986	2164	86
H(1S2)	953	9481	2117	86
H(3)	2596	4837	2764	39
H(2)	2412	4085	3584	42
H(6)	2340	4110	658	34
H(8)	1854	7340	917	40
H(10A)	1787	7870	1826	56
H(10B)	1935	6948	2337	56
H(10C)	1558	6723	1946	56
H(11A)	2452	2418	1316	49
H(11B)	2259	2408	1802	49
H(11C)	2630	3047	1900	49
H(12A)	1959	6955	0	71
H(12B)	2070	5573	-141	71
H(12C)	2357	6576	149	71
H(15)	1552	986	4134	37
H(17)	1206	4592	4133	41
H(19A)	1408	6259	3646	55
H(19B)	1407	5789	3038	55
H(19C)	1764	6025	3486	55
H(20A)	1920	1095	3059	52
H(20B)	1956	365	3631	52
H(20C)	2222	1459	3588	52
H(21A)	877	2352	4401	78
H(21B)	1167	2919	4906	78
H(21C)	1187	1477	4729	78
H(23)	816	5346	2214	30
H(24)	364	4934	2635	40
H(25)	333	2973	3065	43
H(26)	750	1416	3061	37
H(27)	1192	1780	2617	28
H(30)	1772	395	990	33
H(31)	2086	-700	460	37

H(32)	2185	204	-342	42
H(33)	1981	2248	-615	46
H(34)	1686	3393	-75	35
H(36)	935	1362	-4	35
H(37)	912	1386	-957	43
H(38)	698	3164	-1499	46
H(39)	506	4931	-1091	43
H(40)	522	4917	-137	32
H(42)	1132	5437	838	26
H(43)	1025	7598	937	32
H(44)	496	8254	1095	36
H(45)	78	6751	1163	36
H(46)	178	4580	1043	29
H(48)	116	2195	10	40
H(49)	-357	970	94	54
H(50)	-398	281	967	48
H(51)	31	844	1769	42
H(52)	507	2053	1687	32
H(28)	1455(6)	3650(30)	686(11)	25(7)

Table S7. Crystal data and structure refinement for compound **4.**

CCDC deposition number	945574	
Identification code	d12283	
Empirical formula	C52 H49 Cl N2 P2 Ru	
Formula weight	900.39	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.796(3) Å	α = 90°.
	b = 18.979(5) Å	β = 99.625(7)°.
	c = 20.473(5) Å	γ = 90°.
Volume	4519(2) $Å^3$	
Z	4	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	0.514 mm^{-1}	
F(000)	1864	
Crystal size	0.19 x 0.05 x 0.02 mm^3	
Theta range for data collection	1.47 to 27.42°.	
Index ranges	-15<=h<=15, -24<=k<=14, -26<=l<=26	
Reflections collected	40082	
Independent reflections	10285 [R(int) = 0.0505]	
Completeness to theta = 27.42°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10285 / 0 / 523	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0331, wR2 = 0.0675	
R indices (all data)	R1 = 0.0506, wR2 = 0.0736	
Largest diff. peak and hole	0.554 and -0.359 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	5336(2)	723(1)	3082(1)	15(1)
C(2)	5888(2)	-178(1)	3770(1)	24(1)
C(3)	6477(2)	-231(1)	3263(1)	23(1)
C(4)	4479(2)	675(1)	4123(1)	16(1)
C(5)	4942(2)	1194(1)	4568(1)	19(1)
C(6)	4209(2)	1492(1)	4961(1)	21(1)
C(7)	3069(2)	1282(1)	4917(1)	23(1)
C(8)	2675(2)	727(1)	4495(1)	24(1)
C(9)	3370(2)	404(1)	4092(1)	21(1)
C(10)	6164(2)	1448(1)	4622(1)	28(1)
C(11)	2289(3)	1641(1)	5326(1)	39(1)
C(12)	2942(2)	-212(1)	3656(1)	31(1)
C(13)	6660(2)	520(1)	2273(1)	17(1)
C(14)	6515(2)	76(1)	1728(1)	22(1)
C(15)	7078(2)	266(1)	1202(1)	26(1)
C(16)	7744(2)	869(1)	1223(1)	26(1)
C(17)	7852(2)	1307(1)	1778(1)	21(1)
C(18)	7322(2)	1147(1)	2330(1)	16(1)
C(19)	5784(2)	-580(1)	1692(1)	31(1)
C(20)	8380(3)	1051(1)	660(1)	40(1)
C(21)	7388(2)	1624(1)	2898(1)	16(1)
C(22)	3642(2)	1015(1)	2014(1)	21(1)
C(23)	3895(2)	860(1)	1389(1)	26(1)
C(24)	3112(3)	488(2)	932(2)	42(1)
C(25)	2078(3)	268(2)	1095(2)	57(1)
C(26)	1815(3)	421(2)	1714(2)	55(1)
C(27)	2585(2)	798(1)	2171(1)	36(1)
C(28)	5625(2)	2721(1)	3188(1)	17(1)
C(29)	6387(2)	3210(1)	3545(1)	24(1)
C(30)	6140(3)	3551(1)	4106(1)	34(1)
C(31)	5113(3)	3418(1)	4335(1)	36(1)
C(32)	4357(2)	2922(1)	4009(1)	28(1)
C(33)	4611(2)	2564(1)	3453(1)	20(1)
C(34)	3831(2)	1985(1)	3129(1)	18(1)

C(35)	4650(2)	2627(1)	745(1)	20(1)
C(36)	5409(2)	2106(1)	602(1)	24(1)
C(37)	5384(2)	1874(1)	-45(1)	34(1)
C(38)	4623(3)	2166(1)	-560(1)	37(1)
C(39)	3859(2)	2679(1)	-426(1)	35(1)
C(40)	3865(2)	2905(1)	219(1)	27(1)
C(41)	5038(2)	3871(1)	1570(1)	18(1)
C(42)	5065(2)	4244(1)	986(1)	22(1)
C(43)	5308(2)	4967(1)	1009(1)	27(1)
C(44)	5502(2)	5323(1)	1602(1)	29(1)
C(45)	5509(2)	4954(1)	2188(1)	29(1)
C(46)	5289(2)	4232(1)	2174(1)	24(1)
C(47)	3180(2)	2945(1)	1698(1)	24(1)
C(48)	2838(2)	3365(1)	2192(1)	31(1)
C(49)	1705(3)	3340(1)	2313(2)	44(1)
C(50)	904(3)	2900(2)	1946(2)	54(1)
C(51)	1231(2)	2483(2)	1460(2)	46(1)
C(52)	2364(2)	2499(1)	1338(1)	32(1)
Cl(1)	7539(1)	3059(1)	2128(1)	20(1)
N(1)	5187(2)	414(1)	3657(1)	17(1)
N(2)	6136(2)	330(1)	2843(1)	17(1)
P(1)	4699(1)	1514(1)	2601(1)	14(1)
P(2)	4722(1)	2915(1)	1610(1)	16(1)
Ru(1)	6003(1)	2243(1)	2361(1)	13(1)

Table S9. Bond lengths [Å] and angles [°] for compound **4**.

C(1)-N(1)	1.352(3)
C(1)-N(2)	1.355(3)
C(1)-P(1)	1.883(2)
C(2)-C(3)	1.346(3)
C(2)-N(1)	1.391(3)
C(3)-N(2)	1.384(3)
C(4)-C(5)	1.391(3)
C(4)-C(9)	1.397(3)
C(4)-N(1)	1.456(3)
C(5)-C(6)	1.396(3)
C(5)-C(10)	1.506(3)
C(6)-C(7)	1.391(3)
C(7)-C(8)	1.392(3)
C(7)-C(11)	1.507(3)
C(8)-C(9)	1.398(3)
C(9)-C(12)	1.506(3)
C(13)-C(14)	1.386(3)
C(13)-C(18)	1.418(3)
C(13)-N(2)	1.454(3)
C(14)-C(15)	1.404(3)
C(14)-C(19)	1.510(3)
C(15)-C(16)	1.385(3)
C(16)-C(17)	1.396(3)
C(16)-C(20)	1.517(3)
C(17)-C(18)	1.414(3)
C(18)-C(21)	1.466(3)
C(21)-Ru(1)	2.157(2)
C(22)-C(23)	1.393(3)
C(22)-C(27)	1.400(3)
C(22)-P(1)	1.842(2)
C(23)-C(24)	1.391(4)
C(24)-C(25)	1.382(4)
C(25)-C(26)	1.385(4)
C(26)-C(27)	1.389(4)
C(28)-C(29)	1.408(3)
C(28)-C(33)	1.426(3)
C(28)-Ru(1)	2.035(2)

C(29)-C(30)	1.391(3)
C(30)-C(31)	1.393(4)
C(31)-C(32)	1.387(4)
C(32)-C(33)	1.400(3)
C(33)-C(34)	1.514(3)
C(34)-P(1)	1.839(2)
C(35)-C(36)	1.397(3)
C(35)-C(40)	1.400(3)
C(35)-P(2)	1.841(2)
C(36)-C(37)	1.392(3)
C(37)-C(38)	1.381(4)
C(38)-C(39)	1.385(4)
C(39)-C(40)	1.388(3)
C(41)-C(42)	1.394(3)
C(41)-C(46)	1.400(3)
C(41)-P(2)	1.857(2)
C(42)-C(43)	1.401(3)
C(43)-C(44)	1.375(4)
C(44)-C(45)	1.389(3)
C(45)-C(46)	1.394(3)
C(47)-C(52)	1.397(4)
C(47)-C(48)	1.399(3)
C(47)-P(2)	1.859(2)
C(48)-C(49)	1.400(4)
C(49)-C(50)	1.384(5)
C(50)-C(51)	1.377(5)
C(51)-C(52)	1.400(4)
Cl(1)-Ru(1)	2.4899(7)
P(1)-Ru(1)	2.1844(6)
P(2)-Ru(1)	2.3464(7)

N(1)-C(1)-N(2)	105.98(17)
N(1)-C(1)-P(1)	134.54(15)
N(2)-C(1)-P(1)	119.48(15)
C(3)-C(2)-N(1)	107.51(19)
C(2)-C(3)-N(2)	106.70(18)
C(5)-C(4)-C(9)	123.53(19)
C(5)-C(4)-N(1)	117.67(19)
C(9)-C(4)-N(1)	118.78(19)

C(4)-C(5)-C(6)	116.9(2)
C(4)-C(5)-C(10)	122.79(19)
C(6)-C(5)-C(10)	120.3(2)
C(7)-C(6)-C(5)	122.1(2)
C(6)-C(7)-C(8)	118.4(2)
C(6)-C(7)-C(11)	120.5(2)
C(8)-C(7)-C(11)	121.1(2)
C(7)-C(8)-C(9)	122.0(2)
C(4)-C(9)-C(8)	116.7(2)
C(4)-C(9)-C(12)	122.0(2)
C(8)-C(9)-C(12)	121.3(2)
C(14)-C(13)-C(18)	124.64(19)
C(14)-C(13)-N(2)	118.97(18)
C(18)-C(13)-N(2)	116.36(18)
C(13)-C(14)-C(15)	116.9(2)
C(13)-C(14)-C(19)	122.2(2)
C(15)-C(14)-C(19)	120.9(2)
C(16)-C(15)-C(14)	121.7(2)
C(15)-C(16)-C(17)	119.5(2)
C(15)-C(16)-C(20)	121.0(2)
C(17)-C(16)-C(20)	119.5(2)
C(16)-C(17)-C(18)	122.0(2)
C(17)-C(18)-C(13)	115.21(19)
C(17)-C(18)-C(21)	122.00(18)
C(13)-C(18)-C(21)	122.65(18)
C(18)-C(21)-Ru(1)	89.79(13)
C(23)-C(22)-C(27)	119.0(2)
C(23)-C(22)-P(1)	118.82(17)
C(27)-C(22)-P(1)	122.16(19)
C(24)-C(23)-C(22)	120.3(2)
C(25)-C(24)-C(23)	120.3(3)
C(24)-C(25)-C(26)	119.9(3)
C(25)-C(26)-C(27)	120.2(3)
C(26)-C(27)-C(22)	120.2(3)
C(29)-C(28)-C(33)	116.40(19)
C(29)-C(28)-Ru(1)	121.03(16)
C(33)-C(28)-Ru(1)	122.53(16)
C(30)-C(29)-C(28)	122.0(2)
C(29)-C(30)-C(31)	120.5(2)

C(32)-C(31)-C(30)	119.1(2)
C(31)-C(32)-C(33)	120.8(2)
C(32)-C(33)-C(28)	121.0(2)
C(32)-C(33)-C(34)	120.8(2)
C(28)-C(33)-C(34)	118.18(18)
C(33)-C(34)-P(1)	104.67(14)
C(36)-C(35)-C(40)	118.1(2)
C(36)-C(35)-P(2)	118.86(18)
C(40)-C(35)-P(2)	123.02(17)
C(37)-C(36)-C(35)	120.6(2)
C(38)-C(37)-C(36)	120.5(2)
C(37)-C(38)-C(39)	119.5(2)
C(38)-C(39)-C(40)	120.3(2)
C(39)-C(40)-C(35)	120.8(2)
C(42)-C(41)-C(46)	118.48(19)
C(42)-C(41)-P(2)	124.54(17)
C(46)-C(41)-P(2)	116.97(16)
C(41)-C(42)-C(43)	120.2(2)
C(44)-C(43)-C(42)	120.9(2)
C(43)-C(44)-C(45)	119.4(2)
C(44)-C(45)-C(46)	120.2(2)
C(45)-C(46)-C(41)	120.7(2)
C(52)-C(47)-C(48)	118.1(2)
C(52)-C(47)-P(2)	121.96(19)
C(48)-C(47)-P(2)	119.5(2)
C(47)-C(48)-C(49)	120.5(3)
C(50)-C(49)-C(48)	120.7(3)
C(51)-C(50)-C(49)	119.4(3)
C(50)-C(51)-C(52)	120.5(3)
C(47)-C(52)-C(51)	120.8(3)
C(1)-N(1)-C(2)	109.52(17)
C(1)-N(1)-C(4)	126.63(17)
C(2)-N(1)-C(4)	123.70(17)
C(1)-N(2)-C(3)	110.28(17)
C(1)-N(2)-C(13)	124.57(16)
C(3)-N(2)-C(13)	124.76(17)
C(34)-P(1)-C(22)	104.51(10)
C(34)-P(1)-C(1)	107.02(10)
C(22)-P(1)-C(1)	95.67(9)

C(34)-P(1)-Ru(1)	107.88(7)
C(22)-P(1)-Ru(1)	127.16(7)
C(1)-P(1)-Ru(1)	112.78(7)
C(35)-P(2)-C(41)	103.06(9)
C(35)-P(2)-C(47)	102.37(11)
C(41)-P(2)-C(47)	100.45(9)
C(35)-P(2)-Ru(1)	112.97(7)
C(41)-P(2)-Ru(1)	116.63(8)
C(47)-P(2)-Ru(1)	119.07(7)
C(28)-Ru(1)-C(21)	94.09(8)
C(28)-Ru(1)-P(1)	80.51(6)
C(21)-Ru(1)-P(1)	92.48(6)
C(28)-Ru(1)-P(2)	95.52(6)
C(21)-Ru(1)-P(2)	168.55(6)
P(1)-Ru(1)-P(2)	95.21(3)
C(28)-Ru(1)-Cl(1)	98.62(6)
C(21)-Ru(1)-Cl(1)	85.59(6)
P(1)-Ru(1)-Cl(1)	177.83(2)
P(2)-Ru(1)-Cl(1)	86.85(3)

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	15(1)	12(1)	16(1)	-1(1)	2(1)	-3(1)
C(2)	28(1)	19(1)	27(1)	9(1)	7(1)	5(1)
C(3)	26(1)	15(1)	28(1)	4(1)	5(1)	6(1)
C(4)	19(1)	17(1)	14(1)	5(1)	4(1)	1(1)
C(5)	18(1)	21(1)	17(1)	5(1)	2(1)	-3(1)
C(6)	28(1)	21(1)	13(1)	1(1)	2(1)	-2(1)
C(7)	28(1)	24(1)	18(1)	5(1)	9(1)	1(1)
C(8)	18(1)	29(1)	25(1)	4(1)	6(1)	-6(1)
C(9)	24(1)	20(1)	19(1)	3(1)	5(1)	-5(1)
C(10)	21(1)	34(1)	28(2)	-3(1)	3(1)	-9(1)
C(11)	36(2)	49(2)	38(2)	-7(1)	20(1)	-1(1)
C(12)	33(2)	28(1)	33(2)	-6(1)	9(1)	-12(1)
C(13)	17(1)	17(1)	17(1)	1(1)	5(1)	6(1)
C(14)	23(1)	19(1)	24(1)	-2(1)	2(1)	5(1)
C(15)	32(2)	29(1)	18(1)	-7(1)	5(1)	7(1)
C(16)	27(1)	33(1)	18(1)	3(1)	7(1)	9(1)
C(17)	19(1)	22(1)	23(1)	4(1)	5(1)	3(1)
C(18)	13(1)	18(1)	18(1)	3(1)	2(1)	6(1)
C(19)	40(2)	22(1)	30(2)	-7(1)	4(1)	-1(1)
C(20)	45(2)	52(2)	28(2)	0(1)	20(1)	5(1)
C(21)	13(1)	18(1)	17(1)	2(1)	2(1)	1(1)
C(22)	19(1)	20(1)	22(1)	5(1)	-2(1)	-3(1)
C(23)	24(1)	28(1)	24(1)	1(1)	-1(1)	-4(1)
C(24)	43(2)	51(2)	30(2)	-11(1)	-2(1)	-8(1)
C(25)	46(2)	72(2)	47(2)	-17(2)	-10(2)	-28(2)
C(26)	33(2)	79(2)	52(2)	-7(2)	3(2)	-31(2)
C(27)	28(2)	47(2)	32(2)	3(1)	6(1)	-14(1)
C(28)	22(1)	15(1)	14(1)	4(1)	4(1)	1(1)
C(29)	28(1)	25(1)	19(1)	0(1)	6(1)	-6(1)
C(30)	48(2)	31(1)	23(1)	-8(1)	10(1)	-13(1)
C(31)	56(2)	29(1)	30(2)	-10(1)	24(2)	-4(1)
C(32)	37(2)	22(1)	31(2)	2(1)	20(1)	2(1)
C(33)	24(1)	16(1)	21(1)	4(1)	8(1)	4(1)
C(35)	20(1)	17(1)	21(1)	2(1)	1(1)	-4(1)

C(36)	25(1)	21(1)	25(1)	4(1)	1(1)	2(1)
C(37)	45(2)	27(1)	32(2)	-4(1)	8(1)	5(1)
C(38)	50(2)	36(1)	21(1)	-7(1)	0(1)	-4(1)
C(39)	38(2)	40(1)	22(1)	2(1)	-9(1)	1(1)
C(40)	22(1)	31(1)	26(1)	1(1)	-3(1)	2(1)
C(41)	14(1)	16(1)	24(1)	4(1)	3(1)	3(1)
C(42)	19(1)	21(1)	25(1)	4(1)	5(1)	3(1)
C(43)	24(1)	24(1)	33(2)	12(1)	4(1)	0(1)
C(44)	22(1)	19(1)	44(2)	3(1)	2(1)	-2(1)
C(45)	25(1)	26(1)	34(2)	-7(1)	1(1)	-1(1)
C(46)	22(1)	24(1)	24(1)	3(1)	1(1)	0(1)
C(47)	18(1)	23(1)	32(1)	16(1)	4(1)	4(1)
C(48)	29(2)	28(1)	38(2)	16(1)	13(1)	10(1)
C(49)	37(2)	42(1)	61(2)	25(1)	29(2)	18(1)
C(50)	24(2)	58(2)	86(3)	39(2)	24(2)	11(1)
C(51)	20(2)	52(2)	63(2)	27(2)	-1(2)	-5(1)
C(52)	20(1)	36(1)	40(2)	16(1)	0(1)	0(1)
Cl(1)	19(1)	19(1)	25(1)	4(1)	8(1)	-2(1)
N(1)	18(1)	16(1)	18(1)	4(1)	5(1)	0(1)
N(2)	19(1)	14(1)	18(1)	1(1)	5(1)	2(1)
P(1)	14(1)	14(1)	15(1)	2(1)	3(1)	0(1)
P(2)	15(1)	16(1)	18(1)	4(1)	3(1)	1(1)
Ru(1)	13(1)	14(1)	13(1)	2(1)	3(1)	0(1)

References

1 A. J. Arduengo, III, J. C. Calabrese, A. H. Cowley, H. V. R. Dias, J. R. Goerlich, W. J. Marshall and B. Riegel, *Inorg. Chem.*, 1997, **36**, 2151–2158; P. Schwab, R. H. Grubbs and J. W. Ziller, *J. Am. Chem. Soc.*, 1996, **118**, 100–110.

2 APEX, SAINT, SADABS. Bruker AXS, Inc.: Madison, Wisconsin, USA, 2007.

3 L. Palatinus and G. Chapuis, *J. Appl. Crystallogr.*, 2007, **40**, 786–790.

4 L. G. Farrugia, *J. App. Cryst.*, 1999, **32**, 837–838.

5 G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 1990, **A46**, 467–473.