SUPPORTING INFORMATION

Synthesis and *in vitro* (anticancer) evaluation of η^6-arene ruthenium complexes bearing stannyl ligands

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S1. Details for the X-ray Crystallography of C2

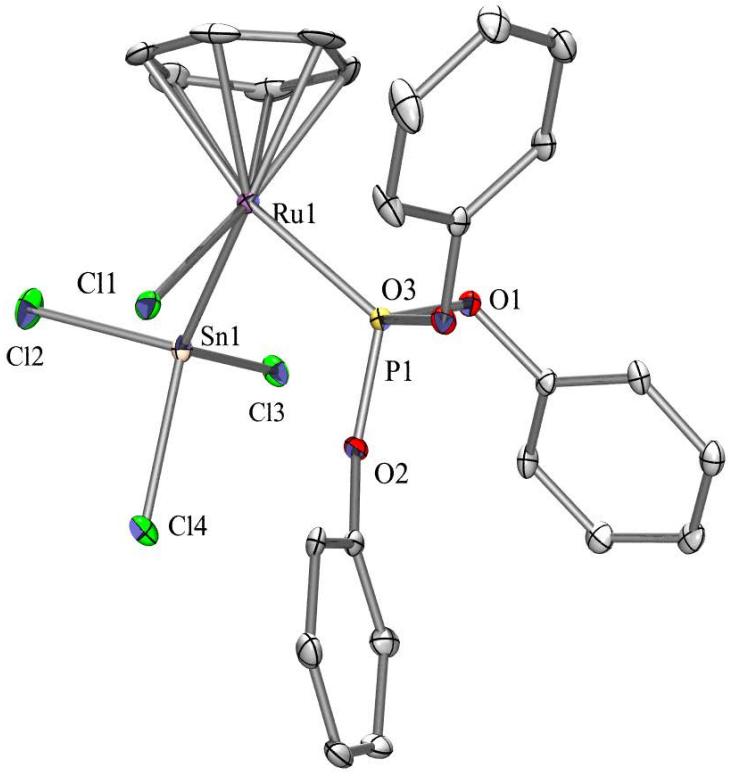

Table S1. Crystal data and structure refinement for *[η^6(C_6H_6)RuCl($SnCl_3$)($P(OPh)_3$)]* ***(C2)***

Empirical formula	C24 H21 Cl4 O3 P Ru Sn
Formula weight	749.94
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 8.7164(17) A alpha = 90 deg. b = 16.420(3) A beta = 90 deg. c = 18.514(4) A gamma = 90 deg.
Volume	2649.9(9) A^3
Z, Calculated density	4, 1.880 Mg/m^3
Absorption coefficient	2.001 mm^-1
F(000)	1464
Crystal size	0.42 x 0.08 x 0.06 mm

Theta range for data collection	1.66 to 26.33 deg.
Limiting indices	-10<=h<=10, -16<=k<=20, -23<=l<=23
Reflections collected / unique	17168 / 5368 [R(int) = 0.0409]
Completeness to theta =	26.33 99.6 %
Absorption correction	SADABS
Max. and min. transmission	0.8893 and 0.4869
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5368 / 0 / 308
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0637
R indices (all data)	R1 = 0.0345, wR2 = 0.0646
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	0.805 and -0.471 e.A^-3

Table S2. Bond lengths [A] and angles [deg]

C(1)-C(2)	1.392(8)
C(1)-C(3)	1.410(9)
C(1)-Ru(1)	2.191(5)
C(2)-C(4)	1.352(8)
C(2)-Ru(1)	2.254(5)
C(3)-C(6)	1.431(9)
C(3)-Ru(1)	2.175(5)
C(4)-C(5)	1.362(8)
C(4)-Ru(1)	2.246(5)
C(5)-C(6)	1.376(8)
C(5)-Ru(1)	2.245(5)
C(6)-Ru(1)	2.249(5)
C(7)-C(10)	1.374(6)
C(7)-C(8)	1.386(6)
C(7)-O(1)	1.408(5)
C(8)-C(9)	1.388(7)
C(9)-C(12)	1.387(7)
C(10)-C(11)	1.386(6)
C(11)-C(12)	1.369(6)

C(13)-C(14)	1.380(6)
C(13)-C(15)	1.384(6)
C(13)-O(2)	1.398(5)
C(14)-C(16)	1.388(6)
C(15)-C(18)	1.385(6)
C(16)-C(17)	1.368(7)
C(17)-C(18)	1.388(7)
C(19)-C(20)	1.367(6)
C(19)-C(24)	1.373(7)
C(20)-C(21)	1.380(6)
C(20)-O(3)	1.409(5)
C(21)-C(22)	1.387(6)
C(22)-C(23)	1.378(7)
C(23)-C(24)	1.368(7)
Cl(1)-Ru(1)	2.3919(10)
Cl(2)-Sn(1)	2.3758(13)
Cl(3)-Sn(1)	2.3750(11)
Cl(4)-Sn(1)	2.3593(12)
O(1)-P(1)	1.606(3)
O(2)-P(1)	1.587(3)
O(3)-P(1)	1.601(3)
P(1)-Ru(1)	2.2442(12)
Ru(1)-Sn(1)	2.5686(5)
C(2)-C(1)-C(3)	118.8(5)
C(2)-C(1)-Ru(1)	74.2(3)
C(3)-C(1)-Ru(1)	70.6(3)
C(4)-C(2)-C(1)	120.5(5)
C(4)-C(2)-Ru(1)	72.2(3)
C(1)-C(2)-Ru(1)	69.3(3)
C(1)-C(3)-C(6)	119.4(5)
C(1)-C(3)-Ru(1)	71.8(3)
C(6)-C(3)-Ru(1)	73.9(3)
C(2)-C(4)-C(5)	121.7(6)
C(2)-C(4)-Ru(1)	72.8(3)
C(5)-C(4)-Ru(1)	72.3(3)
C(4)-C(5)-C(6)	121.0(5)
C(4)-C(5)-Ru(1)	72.4(3)
C(6)-C(5)-Ru(1)	72.3(3)
C(5)-C(6)-C(3)	118.3(5)
C(5)-C(6)-Ru(1)	72.0(3)
C(3)-C(6)-Ru(1)	68.4(3)
C(10)-C(7)-C(8)	121.7(4)
C(10)-C(7)-O(1)	120.6(4)
C(8)-C(7)-O(1)	117.7(4)
C(7)-C(8)-C(9)	118.8(4)
C(12)-C(9)-C(8)	120.1(5)
C(7)-C(10)-C(11)	118.4(4)
C(12)-C(11)-C(10)	121.2(4)
C(11)-C(12)-C(9)	119.8(5)
C(14)-C(13)-C(15)	121.3(4)

C(14)-C(13)-O(2)	123.3(4)
C(15)-C(13)-O(2)	115.2(4)
C(13)-C(14)-C(16)	118.6(4)
C(13)-C(15)-C(18)	118.8(5)
C(17)-C(16)-C(14)	121.3(5)
C(16)-C(17)-C(18)	119.3(5)
C(15)-C(18)-C(17)	120.7(5)
C(20)-C(19)-C(24)	119.4(4)
C(19)-C(20)-C(21)	121.5(4)
C(19)-C(20)-O(3)	118.6(4)
C(21)-C(20)-O(3)	119.9(4)
C(20)-C(21)-C(22)	118.4(4)
C(23)-C(22)-C(21)	120.2(4)
C(24)-C(23)-C(22)	120.1(4)
C(23)-C(24)-C(19)	120.4(5)
C(7)-O(1)-P(1)	120.5(3)
C(13)-O(2)-P(1)	134.7(3)
C(20)-O(3)-P(1)	124.9(3)
O(2)-P(1)-O(3)	99.55(15)
O(2)-P(1)-O(1)	101.65(15)
O(3)-P(1)-O(1)	104.51(15)
O(2)-P(1)-Ru(1)	116.61(12)
O(3)-P(1)-Ru(1)	121.00(12)
O(1)-P(1)-Ru(1)	111.10(12)
C(3)-Ru(1)-C(1)	37.7(2)
C(3)-Ru(1)-P(1)	94.41(16)
C(1)-Ru(1)-P(1)	117.49(18)
C(3)-Ru(1)-C(5)	66.1(2)
C(1)-Ru(1)-C(5)	77.49(19)
P(1)-Ru(1)-C(5)	126.40(17)
C(3)-Ru(1)-C(4)	77.2(2)
C(1)-Ru(1)-C(4)	65.0(2)
P(1)-Ru(1)-C(4)	161.69(16)
C(5)-Ru(1)-C(4)	35.3(2)
C(3)-Ru(1)-C(6)	37.7(2)
C(1)-Ru(1)-C(6)	67.0(2)
P(1)-Ru(1)-C(6)	99.39(16)
C(5)-Ru(1)-C(6)	35.7(2)
C(4)-Ru(1)-C(6)	64.1(2)
C(3)-Ru(1)-C(2)	65.9(2)
C(1)-Ru(1)-C(2)	36.5(2)
P(1)-Ru(1)-C(2)	153.46(16)
C(5)-Ru(1)-C(2)	63.6(2)
C(4)-Ru(1)-C(2)	35.0(2)
C(6)-Ru(1)-C(2)	76.3(2)
C(3)-Ru(1)-Cl(1)	153.5(2)
C(1)-Ru(1)-Cl(1)	156.38(18)
P(1)-Ru(1)-Cl(1)	85.71(4)
C(5)-Ru(1)-Cl(1)	92.60(14)

C(4)-Ru(1)-Cl(1)	94.57(14)
C(6)-Ru(1)-Cl(1)	116.07(19)
C(2)-Ru(1)-Cl(1)	119.96(16)
C(3)-Ru(1)-Sn(1)	122.8(2)
C(1)-Ru(1)-Sn(1)	92.74(15)
P(1)-Ru(1)-Sn(1)	86.84(3)
C(5)-Ru(1)-Sn(1)	146.29(17)
C(4)-Ru(1)-Sn(1)	111.40(15)
C(6)-Ru(1)-Sn(1)	159.53(18)
C(2)-Ru(1)-Sn(1)	89.36(14)
Cl(1)-Ru(1)-Sn(1)	83.67(3)
Cl(4)-Sn(1)-Cl(3)	99.96(4)
Cl(4)-Sn(1)-Cl(2)	96.51(5)
Cl(3)-Sn(1)-Cl(2)	98.09(4)
Cl(4)-Sn(1)-Ru(1)	126.22(3)
Cl(3)-Sn(1)-Ru(1)	116.01(3)
Cl(2)-Sn(1)-Ru(1)	115.03(4)

Table S3. Torsion angles [deg]

C(3)-C(1)-C(2)-C(4)	-3.7(8)
Ru(1)-C(1)-C(2)-C(4)	53.0(5)
C(3)-C(1)-C(2)-Ru(1)	-56.6(4)
C(2)-C(1)-C(3)-C(6)	-0.2(8)
Ru(1)-C(1)-C(3)-C(6)	-58.7(4)
C(2)-C(1)-C(3)-Ru(1)	58.4(4)
C(1)-C(2)-C(4)-C(5)	4.0(8)
Ru(1)-C(2)-C(4)-C(5)	55.7(5)
C(1)-C(2)-C(4)-Ru(1)	-51.7(5)
C(2)-C(4)-C(5)-C(6)	-0.2(8)
Ru(1)-C(4)-C(5)-C(6)	55.7(5)
C(2)-C(4)-C(5)-Ru(1)	-55.9(5)
C(4)-C(5)-C(6)-C(3)	-3.7(8)
Ru(1)-C(5)-C(6)-C(3)	52.0(4)
C(4)-C(5)-C(6)-Ru(1)	-55.7(5)
C(1)-C(3)-C(6)-C(5)	3.8(8)
Ru(1)-C(3)-C(6)-C(5)	-53.8(4)
C(1)-C(3)-C(6)-Ru(1)	57.6(4)
C(10)-C(7)-C(8)-C(9)	1.9(6)
O(1)-C(7)-C(8)-C(9)	-179.3(4)
C(7)-C(8)-C(9)-C(12)	-0.5(7)
C(8)-C(7)-C(10)-C(11)	-1.8(6)
O(1)-C(7)-C(10)-C(11)	179.4(4)
C(7)-C(10)-C(11)-C(12)	0.4(7)
C(10)-C(11)-C(12)-C(9)	0.9(7)
C(8)-C(9)-C(12)-C(11)	-0.8(7)
C(15)-C(13)-C(14)-C(16)	-0.3(7)
O(2)-C(13)-C(14)-C(16)	175.5(4)

C(14)-C(13)-C(15)-C(18)	1.3(7)
O(2)-C(13)-C(15)-C(18)	-174.8(4)
C(13)-C(14)-C(16)-C(17)	-1.2(7)
C(14)-C(16)-C(17)-C(18)	1.7(7)
C(13)-C(15)-C(18)-C(17)	-0.9(7)
C(16)-C(17)-C(18)-C(15)	-0.6(7)
C(24)-C(19)-C(20)-C(21)	-1.0(8)
C(24)-C(19)-C(20)-O(3)	176.0(5)
C(19)-C(20)-C(21)-C(22)	-0.2(7)
O(3)-C(20)-C(21)-C(22)	-177.2(4)
C(20)-C(21)-C(22)-C(23)	1.0(7)
C(21)-C(22)-C(23)-C(24)	-0.7(8)
C(22)-C(23)-C(24)-C(19)	-0.5(9)
C(20)-C(19)-C(24)-C(23)	1.3(9)
C(10)-C(7)-O(1)-P(1)	-88.8(4)
C(8)-C(7)-O(1)-P(1)	92.3(4)
C(14)-C(13)-O(2)-P(1)	37.8(6)
C(15)-C(13)-O(2)-P(1)	-146.2(3)
C(19)-C(20)-O(3)-P(1)	98.9(4)
C(21)-C(20)-O(3)-P(1)	-84.0(5)
C(13)-O(2)-P(1)-O(3)	17.2(4)
C(13)-O(2)-P(1)-O(1)	124.3(4)
C(13)-O(2)-P(1)-Ru(1)	-114.8(4)
C(20)-O(3)-P(1)-O(2)	-159.1(3)
C(20)-O(3)-P(1)-O(1)	96.1(3)
C(20)-O(3)-P(1)-Ru(1)	-30.0(3)
C(7)-O(1)-P(1)-O(2)	-40.7(3)
C(7)-O(1)-P(1)-O(3)	62.5(3)
C(7)-O(1)-P(1)-Ru(1)	-165.4(2)
C(6)-C(3)-Ru(1)-C(1)	129.2(5)
C(1)-C(3)-Ru(1)-P(1)	131.1(3)
C(6)-C(3)-Ru(1)-P(1)	-99.7(3)
C(1)-C(3)-Ru(1)-C(5)	-100.8(4)
C(6)-C(3)-Ru(1)-C(5)	28.4(3)
C(1)-C(3)-Ru(1)-C(4)	-65.4(3)
C(6)-C(3)-Ru(1)-C(4)	63.8(4)
C(1)-C(3)-Ru(1)-C(6)	-129.2(5)
C(1)-C(3)-Ru(1)-C(2)	-30.3(3)
C(6)-C(3)-Ru(1)-C(2)	98.9(4)
C(1)-C(3)-Ru(1)-Cl(1)	-139.6(4)
C(6)-C(3)-Ru(1)-Cl(1)	-10.4(6)
C(1)-C(3)-Ru(1)-Sn(1)	42.1(4)
C(6)-C(3)-Ru(1)-Sn(1)	171.3(3)
C(2)-C(1)-Ru(1)-C(3)	-129.1(5)
C(2)-C(1)-Ru(1)-P(1)	173.1(3)
C(3)-C(1)-Ru(1)-P(1)	-57.8(4)
C(2)-C(1)-Ru(1)-C(5)	-62.2(3)
C(3)-C(1)-Ru(1)-C(5)	66.9(4)
C(2)-C(1)-Ru(1)-C(4)	-27.2(3)
C(3)-C(1)-Ru(1)-C(4)	101.9(4)

C(2)-C(1)-Ru(1)-C(6)	-98.1(4)
C(3)-C(1)-Ru(1)-C(6)	31.0(3)
C(3)-C(1)-Ru(1)-C(2)	129.1(5)
C(2)-C(1)-Ru(1)-Cl(1)	4.8(6)
C(3)-C(1)-Ru(1)-Cl(1)	133.9(4)
C(2)-C(1)-Ru(1)-Sn(1)	85.2(3)
C(3)-C(1)-Ru(1)-Sn(1)	-145.7(3)
O(2)-P(1)-Ru(1)-C(3)	-151.7(2)
O(3)-P(1)-Ru(1)-C(3)	87.1(3)
O(1)-P(1)-Ru(1)-C(3)	-35.9(2)
O(2)-P(1)-Ru(1)-C(1)	-120.5(2)
O(3)-P(1)-Ru(1)-C(1)	118.4(2)
O(1)-P(1)-Ru(1)-C(1)	-4.7(2)
O(2)-P(1)-Ru(1)-C(5)	144.9(2)
O(3)-P(1)-Ru(1)-C(5)	23.8(2)
O(1)-P(1)-Ru(1)-C(5)	-99.3(2)
O(2)-P(1)-Ru(1)-C(4)	146.4(5)
O(3)-P(1)-Ru(1)-C(4)	25.3(5)
O(1)-P(1)-Ru(1)-C(4)	-97.8(5)
O(2)-P(1)-Ru(1)-C(6)	170.6(2)
O(3)-P(1)-Ru(1)-C(6)	49.5(2)
O(1)-P(1)-Ru(1)-C(6)	-73.6(2)
O(2)-P(1)-Ru(1)-C(2)	-111.2(3)
O(3)-P(1)-Ru(1)-C(2)	127.6(3)
O(1)-P(1)-Ru(1)-C(2)	4.6(3)
O(2)-P(1)-Ru(1)-Cl(1)	54.86(12)
O(3)-P(1)-Ru(1)-Cl(1)	-66.29(13)
O(1)-P(1)-Ru(1)-Cl(1)	170.68(12)
O(2)-P(1)-Ru(1)-Sn(1)	-29.02(12)
O(3)-P(1)-Ru(1)-Sn(1)	-150.17(13)
O(1)-P(1)-Ru(1)-Sn(1)	86.80(12)
C(4)-C(5)-Ru(1)-C(3)	102.0(4)
C(6)-C(5)-Ru(1)-C(3)	-30.0(4)
C(4)-C(5)-Ru(1)-C(1)	64.1(4)
C(6)-C(5)-Ru(1)-C(1)	-67.9(4)
C(4)-C(5)-Ru(1)-P(1)	179.2(3)
C(6)-C(5)-Ru(1)-P(1)	47.2(4)
C(6)-C(5)-Ru(1)-C(4)	-132.0(5)
C(4)-C(5)-Ru(1)-C(6)	132.0(5)
C(4)-C(5)-Ru(1)-C(2)	28.2(3)
C(6)-C(5)-Ru(1)-C(2)	-103.9(4)
C(4)-C(5)-Ru(1)-Cl(1)	-94.2(3)
C(6)-C(5)-Ru(1)-Cl(1)	133.7(3)
C(4)-C(5)-Ru(1)-Sn(1)	-11.7(5)
C(6)-C(5)-Ru(1)-Sn(1)	-143.8(3)
C(2)-C(4)-Ru(1)-C(3)	66.1(4)
C(5)-C(4)-Ru(1)-C(3)	-66.4(4)
C(2)-C(4)-Ru(1)-C(1)	28.3(3)
C(5)-C(4)-Ru(1)-C(1)	-104.2(4)
C(2)-C(4)-Ru(1)-P(1)	130.4(4)

C(5)-C(4)-Ru(1)-P(1)	-2.1(7)
C(2)-C(4)-Ru(1)-C(5)	132.5(5)
C(2)-C(4)-Ru(1)-C(6)	103.7(4)
C(5)-C(4)-Ru(1)-C(6)	-28.8(3)
C(5)-C(4)-Ru(1)-C(2)	-132.5(5)
C(2)-C(4)-Ru(1)-Cl(1)	-139.4(3)
C(5)-C(4)-Ru(1)-Cl(1)	88.0(3)
C(2)-C(4)-Ru(1)-Sn(1)	-54.5(3)
C(5)-C(4)-Ru(1)-Sn(1)	173.0(3)
C(5)-C(6)-Ru(1)-C(3)	131.7(5)
C(5)-C(6)-Ru(1)-C(1)	100.8(4)
C(3)-C(6)-Ru(1)-C(1)	-30.9(3)
C(5)-C(6)-Ru(1)-P(1)	-143.3(3)
C(3)-C(6)-Ru(1)-P(1)	85.0(3)
C(3)-C(6)-Ru(1)-C(5)	-131.7(5)
C(5)-C(6)-Ru(1)-C(4)	28.5(3)
C(3)-C(6)-Ru(1)-C(4)	-103.2(4)
C(5)-C(6)-Ru(1)-C(2)	63.5(4)
C(3)-C(6)-Ru(1)-C(2)	-68.2(4)
C(5)-C(6)-Ru(1)-Cl(1)	-53.5(4)
C(3)-C(6)-Ru(1)-Cl(1)	174.8(3)
C(5)-C(6)-Ru(1)-Sn(1)	110.3(6)
C(3)-C(6)-Ru(1)-Sn(1)	-21.4(7)
C(4)-C(2)-Ru(1)-C(3)	-102.5(4)
C(1)-C(2)-Ru(1)-C(3)	31.3(3)
C(4)-C(2)-Ru(1)-C(1)	-133.8(5)
C(4)-C(2)-Ru(1)-P(1)	-147.6(3)
C(1)-C(2)-Ru(1)-P(1)	-13.9(5)
C(4)-C(2)-Ru(1)-C(5)	-28.4(3)
C(1)-C(2)-Ru(1)-C(5)	105.4(4)
C(1)-C(2)-Ru(1)-C(4)	133.8(5)
C(4)-C(2)-Ru(1)-C(6)	-64.0(4)
C(1)-C(2)-Ru(1)-C(6)	69.7(4)
C(4)-C(2)-Ru(1)-Cl(1)	48.4(4)
C(1)-C(2)-Ru(1)-Cl(1)	-177.8(3)
C(4)-C(2)-Ru(1)-Sn(1)	130.7(3)
C(1)-C(2)-Ru(1)-Sn(1)	-95.5(3)
C(3)-Ru(1)-Sn(1)-Cl(4)	148.83(19)
C(1)-Ru(1)-Sn(1)-Cl(4)	173.02(18)
P(1)-Ru(1)-Sn(1)-Cl(4)	55.62(5)
C(5)-Ru(1)-Sn(1)-Cl(4)	-115.6(2)
C(4)-Ru(1)-Sn(1)-Cl(4)	-122.85(15)
C(6)-Ru(1)-Sn(1)-Cl(4)	164.2(5)
C(2)-Ru(1)-Sn(1)-Cl(4)	-150.65(16)
Cl(1)-Ru(1)-Sn(1)-Cl(4)	-30.40(5)
C(3)-Ru(1)-Sn(1)-Cl(3)	22.25(19)
C(1)-Ru(1)-Sn(1)-Cl(3)	46.44(18)
P(1)-Ru(1)-Sn(1)-Cl(3)	-70.96(4)
C(5)-Ru(1)-Sn(1)-Cl(3)	117.8(2)
C(4)-Ru(1)-Sn(1)-Cl(3)	110.57(15)

C(6)-Ru(1)-Sn(1)-Cl(3)	37.7(5)
C(2)-Ru(1)-Sn(1)-Cl(3)	82.76(16)
Cl(1)-Ru(1)-Sn(1)-Cl(3)	-156.99(5)
C(3)-Ru(1)-Sn(1)-Cl(2)	-91.36(19)
C(1)-Ru(1)-Sn(1)-Cl(2)	-67.17(18)
P(1)-Ru(1)-Sn(1)-Cl(2)	175.42(5)
C(5)-Ru(1)-Sn(1)-Cl(2)	4.2(3)
C(4)-Ru(1)-Sn(1)-Cl(2)	-3.04(15)
C(6)-Ru(1)-Sn(1)-Cl(2)	-76.0(5)
C(2)-Ru(1)-Sn(1)-Cl(2)	-30.85(16)
Cl(1)-Ru(1)-Sn(1)-Cl(2)	89.40(5)

S2. Details for the X-ray Crystallography of $[(\eta^6\text{-}C_6H_6)RuCl_2P(OPh)_3]$

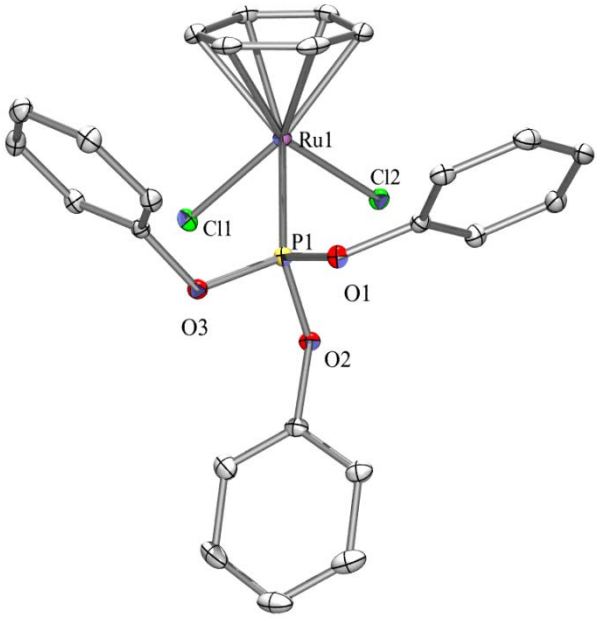

Table S4. Crystal data and structure refinement for $[(\eta^6\text{-}C_6H_6)RuCl_2P(OPh)_3]$

Empirical formula	C24 H21 Cl2 O3 P Ru
Formula weight	560.35
Temperature	446(2) K
Wavelength	0.71073 A
Crystal system, space group	orthorhombic, Pbca
Unit cell dimensions	a = 17.371(3) A alpha = 90 deg. b = 14.997(3) A beta = 90 deg. c = 17.551(3) A gamma = 90 deg.
Volume	4572.6(14) A^3
Z, Calculated density	8, 1.628 Mg/m^3
Absorption coefficient	1.013 mm^-1
F(000)	2256
Crystal size	0.38 x 0.36 x 0.16 mm

Theta range for data collection	2.14 to 26.34 deg.
Limiting indices	-21<=h<=21, -18<=k<=18, -21<=l<=21
Reflections collected / unique	34691 / 4657 [R(int) = 0.0339]
Completeness to theta =	26.34 99.9 %
Absorption correction	SADABS
Max. and min. transmission	0.8547 and 0.6994
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4657 / 0 / 280
Goodness-of-fit on F^2	1.117
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0652
R indices (all data)	R1 = 0.0322, wR2 = 0.0665
Largest diff. peak and hole	0.566 and -0.404 e.A^-3

Table S5. Bond lengths [A] and angles [deg]

Ru(1)-C(23)	2.178(2)
Ru(1)-C(24)	2.189(2)
Ru(1)-C(19)	2.194(2)
Ru(1)-C(21)	2.216(2)
Ru(1)-C(22)	2.249(2)
Ru(1)-C(20)	2.261(2)
Ru(1)-P(1)	2.2689(7)
Ru(1)-Cl(2)	2.4058(7)
Ru(1)-Cl(1)	2.4099(7)
P(1)-O(2)	1.5874(16)
P(1)-O(3)	1.5994(16)
P(1)-O(1)	1.6147(16)
O(1)-C(1)	1.405(3)
O(2)-C(7)	1.409(3)
O(3)-C(13)	1.408(3)
C(5)-C(4)	1.383(4)
C(5)-C(6)	1.388(4)
C(6)-C(1)	1.385(3)
C(23)-C(24)	1.396(4)
C(23)-C(22)	1.424(4)
C(14)-C(13)	1.381(3)
C(14)-C(15)	1.387(3)

C(19)-C(21)	1.397(4)
C(19)-C(20)	1.422(3)
C(16)-C(13)	1.382(3)
C(16)-C(18)	1.393(3)
C(2)-C(1)	1.379(3)
C(2)-C(3)	1.393(4)
C(3)-C(4)	1.384(4)
C(12)-C(7)	1.381(3)
C(12)-C(11)	1.395(4)
C(20)-C(22)	1.377(4)
C(21)-C(24)	1.412(4)
C(7)-C(8)	1.374(3)
C(10)-C(11)	1.375(4)
C(10)-C(9)	1.381(4)
C(8)-C(9)	1.398(4)
C(15)-C(17)	1.385(3)
C(18)-C(17)	1.388(3)
C(23)-Ru(1)-C(24)	37.30(11)
C(23)-Ru(1)-C(19)	79.68(9)
C(24)-Ru(1)-C(19)	67.19(10)
C(23)-Ru(1)-C(21)	67.30(10)
C(24)-Ru(1)-C(21)	37.38(10)
C(19)-Ru(1)-C(21)	36.93(9)
C(23)-Ru(1)-C(22)	37.48(10)
C(24)-Ru(1)-C(22)	66.59(10)
C(19)-Ru(1)-C(22)	65.93(9)
C(21)-Ru(1)-C(22)	78.00(9)
C(23)-Ru(1)-C(20)	66.44(10)
C(24)-Ru(1)-C(20)	78.43(9)
C(19)-Ru(1)-C(20)	37.19(9)
C(21)-Ru(1)-C(20)	66.26(9)
C(22)-Ru(1)-C(20)	35.56(10)
C(23)-Ru(1)-P(1)	117.63(8)
C(24)-Ru(1)-P(1)	94.20(7)
C(19)-Ru(1)-P(1)	123.29(7)
C(21)-Ru(1)-P(1)	96.90(6)
C(22)-Ru(1)-P(1)	154.72(7)
C(20)-Ru(1)-P(1)	160.48(7)
C(23)-Ru(1)-Cl(2)	91.38(7)
C(24)-Ru(1)-Cl(2)	122.33(8)
C(19)-Ru(1)-Cl(2)	145.01(7)
C(21)-Ru(1)-Cl(2)	158.56(7)
C(22)-Ru(1)-Cl(2)	86.43(7)
C(20)-Ru(1)-Cl(2)	108.36(6)
P(1)-Ru(1)-Cl(2)	90.90(2)
C(23)-Ru(1)-Cl(1)	160.64(8)
C(24)-Ru(1)-Cl(1)	150.06(8)
C(19)-Ru(1)-Cl(1)	90.23(7)
C(21)-Ru(1)-Cl(1)	113.34(7)
C(22)-Ru(1)-Cl(1)	123.20(7)

C(20)-Ru(1)-Cl(1)	95.60(7)
P(1)-Ru(1)-Cl(1)	81.72(2)
Cl(2)-Ru(1)-Cl(1)	87.49(2)
O(2)-P(1)-O(3)	100.19(8)
O(2)-P(1)-O(1)	105.02(9)
O(3)-P(1)-O(1)	96.90(8)
O(2)-P(1)-Ru(1)	114.54(6)
O(3)-P(1)-Ru(1)	118.38(6)
O(1)-P(1)-Ru(1)	118.81(6)
C(1)-O(1)-P(1)	124.00(14)
C(7)-O(2)-P(1)	124.81(13)
C(13)-O(3)-P(1)	121.26(13)
C(4)-C(5)-C(6)	120.2(2)
C(1)-C(6)-C(5)	118.7(2)
C(24)-C(23)-C(22)	119.5(2)
C(24)-C(23)-Ru(1)	71.79(14)
C(22)-C(23)-Ru(1)	73.97(14)
C(13)-C(14)-C(15)	118.6(2)
C(21)-C(19)-C(20)	120.5(2)
C(21)-C(19)-Ru(1)	72.38(14)
C(20)-C(19)-Ru(1)	73.94(14)
C(13)-C(16)-C(18)	118.6(2)
C(14)-C(13)-C(16)	122.2(2)
C(14)-C(13)-O(3)	118.1(2)
C(16)-C(13)-O(3)	119.6(2)
C(1)-C(2)-C(3)	118.5(2)
C(4)-C(3)-C(2)	120.3(2)
C(7)-C(12)-C(11)	118.9(3)
C(22)-C(20)-C(19)	119.5(2)
C(22)-C(20)-Ru(1)	71.73(14)
C(19)-C(20)-Ru(1)	68.86(13)
C(5)-C(4)-C(3)	120.3(2)
C(19)-C(21)-C(24)	119.4(2)
C(19)-C(21)-Ru(1)	70.69(14)
C(24)-C(21)-Ru(1)	70.26(14)
C(8)-C(7)-C(12)	122.1(2)
C(8)-C(7)-O(2)	119.0(2)
C(12)-C(7)-O(2)	118.7(2)
C(11)-C(10)-C(9)	120.5(3)
C(23)-C(24)-C(21)	120.2(2)
C(23)-C(24)-Ru(1)	70.91(14)
C(21)-C(24)-Ru(1)	72.35(14)
C(10)-C(11)-C(12)	119.8(3)
C(7)-C(8)-C(9)	118.3(3)
C(10)-C(9)-C(8)	120.4(3)
C(2)-C(1)-C(6)	122.0(2)
C(2)-C(1)-O(1)	122.0(2)
C(6)-C(1)-O(1)	116.0(2)
C(17)-C(15)-C(14)	120.4(2)
C(20)-C(22)-C(23)	120.6(2)

C(20)-C(22)-Ru(1)	72.70(14)
C(23)-C(22)-Ru(1)	68.55(14)
C(17)-C(18)-C(16)	119.9(2)
C(15)-C(17)-C(18)	120.3(2)

Table S6. Torsion angles [deg]

C(23)-Ru(1)-P(1)-O(2)	-118.65(11)
C(24)-Ru(1)-P(1)-O(2)	-149.13(10)
C(19)-Ru(1)-P(1)-O(2)	145.51(10)
C(21)-Ru(1)-P(1)-O(2)	173.40(10)
C(22)-Ru(1)-P(1)-O(2)	-110.15(17)
C(20)-Ru(1)-P(1)-O(2)	144.1(2)
Cl(2)-Ru(1)-P(1)-O(2)	-26.62(7)
Cl(1)-Ru(1)-P(1)-O(2)	60.72(7)
C(23)-Ru(1)-P(1)-O(3)	123.46(10)
C(24)-Ru(1)-P(1)-O(3)	92.98(10)
C(19)-Ru(1)-P(1)-O(3)	27.62(11)
C(21)-Ru(1)-P(1)-O(3)	55.51(10)
C(22)-Ru(1)-P(1)-O(3)	131.96(16)
C(20)-Ru(1)-P(1)-O(3)	26.2(2)
Cl(2)-Ru(1)-P(1)-O(3)	-144.51(7)
Cl(1)-Ru(1)-P(1)-O(3)	-57.17(7)
C(23)-Ru(1)-P(1)-O(1)	6.53(11)
C(24)-Ru(1)-P(1)-O(1)	-23.95(10)
C(19)-Ru(1)-P(1)-O(1)	-89.31(11)
C(21)-Ru(1)-P(1)-O(1)	-61.42(10)
C(22)-Ru(1)-P(1)-O(1)	15.03(17)
C(20)-Ru(1)-P(1)-O(1)	-90.7(2)
Cl(2)-Ru(1)-P(1)-O(1)	98.56(7)
Cl(1)-Ru(1)-P(1)-O(1)	-174.10(7)
O(2)-P(1)-O(1)-C(1)	85.37(17)
O(3)-P(1)-O(1)-C(1)	-172.10(16)
Ru(1)-P(1)-O(1)-C(1)	-44.30(18)
O(3)-P(1)-O(2)-C(7)	-35.78(19)
O(1)-P(1)-O(2)-C(7)	64.28(19)
Ru(1)-P(1)-O(2)-C(7)	-163.58(15)
O(2)-P(1)-O(3)-C(13)	-169.67(16)
O(1)-P(1)-O(3)-C(13)	83.65(16)
Ru(1)-P(1)-O(3)-C(13)	-44.45(17)
C(4)-C(5)-C(6)-C(1)	-0.5(3)
C(19)-Ru(1)-C(23)-C(24)	65.72(15)
C(21)-Ru(1)-C(23)-C(24)	29.28(14)
C(22)-Ru(1)-C(23)-C(24)	129.4(2)
C(20)-Ru(1)-C(23)-C(24)	102.21(16)
P(1)-Ru(1)-C(23)-C(24)	-56.59(16)
Cl(2)-Ru(1)-C(23)-C(24)	-148.33(14)
Cl(1)-Ru(1)-C(23)-C(24)	125.3(2)
C(24)-Ru(1)-C(23)-C(22)	-129.4(2)

C(19)-Ru(1)-C(23)-C(22)	-63.65(15)
C(21)-Ru(1)-C(23)-C(22)	-100.09(16)
C(20)-Ru(1)-C(23)-C(22)	-27.16(14)
P(1)-Ru(1)-C(23)-C(22)	174.04(12)
Cl(2)-Ru(1)-C(23)-C(22)	82.30(14)
Cl(1)-Ru(1)-C(23)-C(22)	-4.1(3)
C(23)-Ru(1)-C(19)-C(21)	-65.76(16)
C(24)-Ru(1)-C(19)-C(21)	-28.94(15)
C(22)-Ru(1)-C(19)-C(21)	-102.43(17)
C(20)-Ru(1)-C(19)-C(21)	-130.2(2)
P(1)-Ru(1)-C(19)-C(21)	50.62(16)
Cl(2)-Ru(1)-C(19)-C(21)	-143.20(13)
Cl(1)-Ru(1)-C(19)-C(21)	130.85(14)
C(23)-Ru(1)-C(19)-C(20)	64.39(16)
C(24)-Ru(1)-C(19)-C(20)	101.21(16)
C(21)-Ru(1)-C(19)-C(20)	130.2(2)
C(22)-Ru(1)-C(19)-C(20)	27.73(14)
P(1)-Ru(1)-C(19)-C(20)	-179.22(12)
Cl(2)-Ru(1)-C(19)-C(20)	-13.0(2)
Cl(1)-Ru(1)-C(19)-C(20)	-99.00(14)
C(15)-C(14)-C(13)-C(16)	1.0(3)
C(15)-C(14)-C(13)-O(3)	178.58(19)
C(18)-C(16)-C(13)-C(14)	0.1(3)
C(18)-C(16)-C(13)-O(3)	-177.42(19)
P(1)-O(3)-C(13)-C(14)	100.7(2)
P(1)-O(3)-C(13)-C(16)	-81.7(2)
C(1)-C(2)-C(3)-C(4)	0.9(3)
C(21)-C(19)-C(20)-C(22)	4.9(3)
Ru(1)-C(19)-C(20)-C(22)	-52.8(2)
C(21)-C(19)-C(20)-Ru(1)	57.7(2)
C(23)-Ru(1)-C(20)-C(22)	28.52(15)
C(24)-Ru(1)-C(20)-C(22)	65.72(16)
C(19)-Ru(1)-C(20)-C(22)	133.1(2)
C(21)-Ru(1)-C(20)-C(22)	102.97(16)
P(1)-Ru(1)-C(20)-C(22)	135.02(19)
Cl(2)-Ru(1)-C(20)-C(22)	-54.76(15)
Cl(1)-Ru(1)-C(20)-C(22)	-143.97(14)
C(23)-Ru(1)-C(20)-C(19)	-104.56(17)
C(24)-Ru(1)-C(20)-C(19)	-67.36(16)
C(21)-Ru(1)-C(20)-C(19)	-30.11(15)
C(22)-Ru(1)-C(20)-C(19)	-133.1(2)
P(1)-Ru(1)-C(20)-C(19)	1.9(3)
Cl(2)-Ru(1)-C(20)-C(19)	172.16(13)
Cl(1)-Ru(1)-C(20)-C(19)	82.95(14)
C(6)-C(5)-C(4)-C(3)	0.8(4)
C(2)-C(3)-C(4)-C(5)	-1.0(4)
C(20)-C(19)-C(21)-C(24)	-5.9(3)
Ru(1)-C(19)-C(21)-C(24)	52.5(2)
C(20)-C(19)-C(21)-Ru(1)	-58.4(2)
C(23)-Ru(1)-C(21)-C(19)	103.49(17)

C(24)-Ru(1)-C(21)-C(19)	132.7(2)
C(22)-Ru(1)-C(21)-C(19)	65.72(16)
C(20)-Ru(1)-C(21)-C(19)	30.31(15)
P(1)-Ru(1)-C(21)-C(19)	-139.40(14)
Cl(2)-Ru(1)-C(21)-C(19)	110.0(2)
Cl(1)-Ru(1)-C(21)-C(19)	-55.47(15)
C(23)-Ru(1)-C(21)-C(24)	-29.22(15)
C(19)-Ru(1)-C(21)-C(24)	-132.7(2)
C(22)-Ru(1)-C(21)-C(24)	-66.99(15)
C(20)-Ru(1)-C(21)-C(24)	-102.40(16)
P(1)-Ru(1)-C(21)-C(24)	87.89(14)
Cl(2)-Ru(1)-C(21)-C(24)	-22.7(3)
Cl(1)-Ru(1)-C(21)-C(24)	171.82(12)
C(11)-C(12)-C(7)-C(8)	-0.8(3)
C(11)-C(12)-C(7)-O(2)	-175.8(2)
P(1)-O(2)-C(7)-C(8)	89.0(2)
P(1)-O(2)-C(7)-C(12)	-95.8(2)
C(22)-C(23)-C(24)-C(21)	3.6(3)
Ru(1)-C(23)-C(24)-C(21)	-55.1(2)
C(22)-C(23)-C(24)-Ru(1)	58.6(2)
C(19)-C(21)-C(24)-C(23)	1.6(3)
Ru(1)-C(21)-C(24)-C(23)	54.4(2)
C(19)-C(21)-C(24)-Ru(1)	-52.7(2)
C(19)-Ru(1)-C(24)-C(23)	-103.38(16)
C(21)-Ru(1)-C(24)-C(23)	-132.0(2)
C(22)-Ru(1)-C(24)-C(23)	-30.84(15)
C(20)-Ru(1)-C(24)-C(23)	-66.13(15)
P(1)-Ru(1)-C(24)-C(23)	132.14(14)
Cl(2)-Ru(1)-C(24)-C(23)	38.40(16)
Cl(1)-Ru(1)-C(24)-C(23)	-147.17(14)
C(23)-Ru(1)-C(24)-C(21)	132.0(2)
C(19)-Ru(1)-C(24)-C(21)	28.62(14)
C(22)-Ru(1)-C(24)-C(21)	101.16(16)
C(20)-Ru(1)-C(24)-C(21)	65.87(15)
P(1)-Ru(1)-C(24)-C(21)	-95.87(14)
Cl(2)-Ru(1)-C(24)-C(21)	170.40(12)
Cl(1)-Ru(1)-C(24)-C(21)	-15.2(2)
C(9)-C(10)-C(11)-C(12)	1.4(4)
C(7)-C(12)-C(11)-C(10)	-0.8(4)
C(12)-C(7)-C(8)-C(9)	1.6(4)
O(2)-C(7)-C(8)-C(9)	176.7(2)
C(11)-C(10)-C(9)-C(8)	-0.5(4)
C(7)-C(8)-C(9)-C(10)	-1.0(4)
C(3)-C(2)-C(1)-C(6)	-0.7(3)
C(3)-C(2)-C(1)-O(1)	-179.1(2)
C(5)-C(6)-C(1)-C(2)	0.5(3)
C(5)-C(6)-C(1)-O(1)	179.00(19)
P(1)-O(1)-C(1)-C(2)	-39.9(3)
P(1)-O(1)-C(1)-C(6)	141.56(17)
C(13)-C(14)-C(15)-C(17)	-1.1(3)

C(19)-C(20)-C(22)-C(23)	0.4(3)
Ru(1)-C(20)-C(22)-C(23)	-51.0(2)
C(19)-C(20)-C(22)-Ru(1)	51.5(2)
C(24)-C(23)-C(22)-C(20)	-4.6(4)
Ru(1)-C(23)-C(22)-C(20)	52.9(2)
C(24)-C(23)-C(22)-Ru(1)	-57.6(2)
C(23)-Ru(1)-C(22)-C(20)	-134.0(2)
C(24)-Ru(1)-C(22)-C(20)	-103.30(16)
C(19)-Ru(1)-C(22)-C(20)	-28.92(14)
C(21)-Ru(1)-C(22)-C(20)	-65.78(15)
P(1)-Ru(1)-C(22)-C(20)	-146.42(14)
Cl(2)-Ru(1)-C(22)-C(20)	129.04(14)
Cl(1)-Ru(1)-C(22)-C(20)	44.39(16)
C(24)-Ru(1)-C(22)-C(23)	30.70(15)
C(19)-Ru(1)-C(22)-C(23)	105.08(17)
C(21)-Ru(1)-C(22)-C(23)	68.21(16)
C(20)-Ru(1)-C(22)-C(23)	134.0(2)
P(1)-Ru(1)-C(22)-C(23)	-12.4(3)
Cl(2)-Ru(1)-C(22)-C(23)	-96.96(15)
Cl(1)-Ru(1)-C(22)-C(23)	178.39(13)
C(13)-C(16)-C(18)-C(17)	-1.2(3)
C(14)-C(15)-C(17)-C(18)	0.0(4)
C(16)-C(18)-C(17)-C(15)	1.1(4)