Crystallographic Data

$[K(C_{10}H_{10}O_5)_2][Ir(Cl)\{N(CHCHP\mathit{t}Bu_2)_2\}]$ (3)

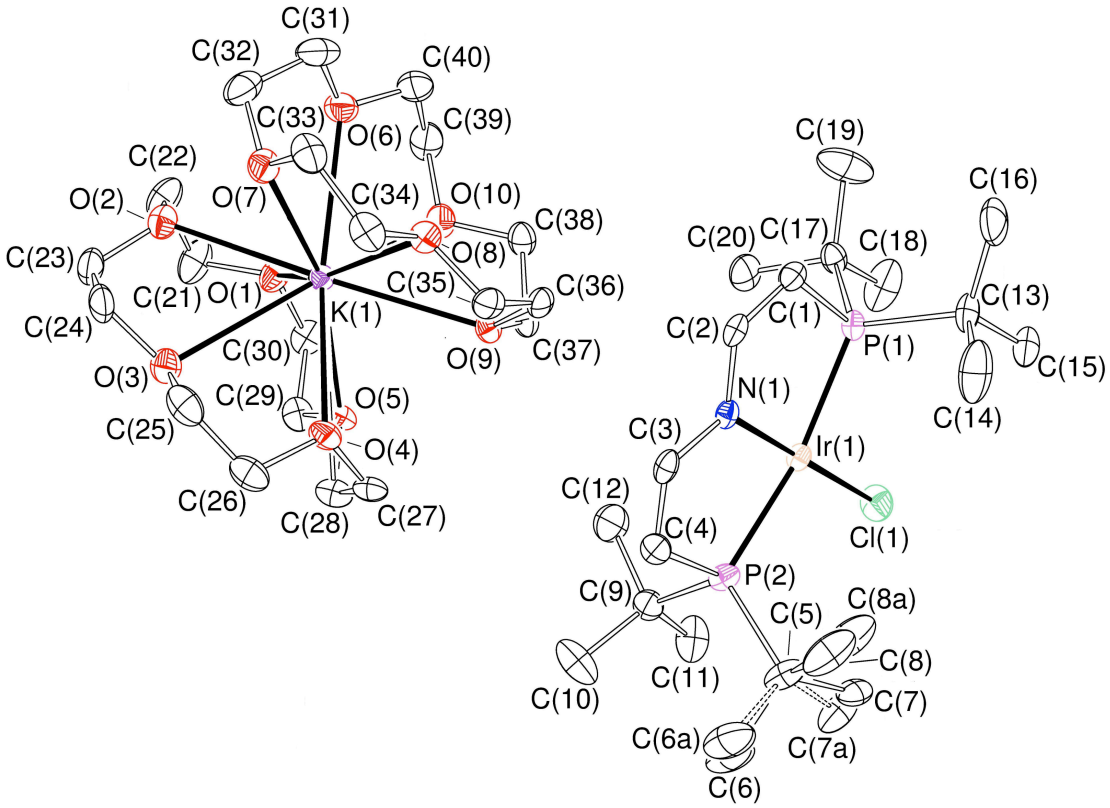

Figure S1. ORTEP plot of **3** with the anisotropic displacement parameters drawn at the 50% probability level. The hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for **3**.

CCDC no.	967913	
Empirical formula	$C_{40}H_{80}ClIrKNO_{10}P_2$	
Formula weight	1063.74 g/mol	
Temperature	100(2) K	
Wavelength	0.56086 Å	
Crystal system	Orthorhombic	
Space group	Pbcn	
Unit cell dimensions	a = 20.279(2) Å	α= 90°
	b = 18.474(2) Å	β= 90°
	c = 26.694(3) Å	γ = 90°
Volume	10000.5(18) $Å^3$	
Z	8	

Density (calculated)	1.413 Mg/m^3	
Absorption coefficient	1.586 mm^{-1}	
F(000)	4400	
Crystal size	0.103 x 0.103 x 0.097 mm^3	
Theta range for data collection	1.684 to 19.796°	
Index ranges	-20<=h<=24, -21<=k<=22, -32<=l<=26	
Reflections collected	156766	
Independent reflections	9180 [R(int) = 0.0808]	
Completeness to theta = 19.665°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7444 and 0.6855	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9180 / 156 / 539	
Goodness-of-fit on F^2	1.000	
Final R indices [I>2sigma(I)]	R1 = 0.0261,	wR2 = 0.0420
R indices (all data)	R1 = 0.0492,	wR2 = 0.0483
Largest diff. peak and hole	0.645 and -0.677 $eÅ^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for **3**.

Ir(1)-N(1)	2.030(2)	O(5)-K(1)-O(3)	82.77(6)
Ir(1)-P(2)	2.2760(9)	O(10)-K(1)-O(3)	128.78(7)
Ir(1)-P(1)	2.2779(9)	O(2)-K(1)-O(3)	57.63(7)
Ir(1)-Cl(1)	2.3995(8)	O(11)-K(1)-O(3)	157.96(7)
K(1)-O(7)	2.828(2)	O(9)-K(1)-O(3)	107.41(6)
K(1)-O(4)	2.835(2)	O(7)-K(1)-C(32)	42.34(8)
K(1)-O(8)	2.837(2)	O(4)-K(1)-C(32)	124.29(8)
K(1)-O(1)	2.838(2)	O(8)-K(1)-C(32)	22.76(7)
K(1)-O(5)	2.843(2)	O(1)-K(1)-C(32)	106.25(8)
K(1)-O(10)	2.843(2)	O(5)-K(1)-C(32)	164.06(8)
K(1)-O(2)	2.849(2)	O(10)-K(1)-C(32)	122.61(8)
K(1)-O(11)	2.905(2)	O(2)-K(1)-C(32)	60.40(8)
K(1)-O(9)	2.960(2)	O(11)-K(1)-C(32)	102.93(8)
K(1)-O(3)	3.003(2)	O(9)-K(1)-C(32)	71.36(7)
K(1)-C(32)	3.533(3)	O(3)-K(1)-C(32)	89.02(8)

P(1)-C(1)	1.786(3)	C(1)-P(1)-C(17)	103.88(15)
P(1)-C(17)	1.879(3)	C(1)-P(1)-C(13)	102.98(15)
P(1)-C(13)	1.889(3)	C(17)-P(1)-C(13)	110.44(15)
O(1)-C(21)	1.423(4)	C(1)-P(1)-Ir(1)	101.73(11)
O(1)-C(30)	1.430(4)	C(17)-P(1)-Ir(1)	118.04(10)
O(2)-C(22)	1.419(4)	C(13)-P(1)-Ir(1)	117.10(11)
O(2)-C(23)	1.423(4)	C(21)-O(1)-C(30)	113.4(3)
O(3)-C(24)	1.420(4)	C(21)-O(1)-K(1)	117.24(19)
O(3)-C(25)	1.422(4)	C(30)-O(1)-K(1)	112.71(18)
O(4)-C(27)	1.428(4)	C(22)-O(2)-C(23)	114.2(3)
O(4)-C(26)	1.429(4)	C(22)-O(2)-K(1)	110.36(19)
O(5)-C(29)	1.415(4)	C(23)-O(2)-K(1)	120.25(19)
O(5)-C(28)	1.425(4)	C(24)-O(3)-C(25)	112.4(3)
O(7)-C(40)	1.420(4)	C(24)-O(3)-K(1)	106.82(19)
O(7)-C(31)	1.428(4)	C(25)-O(3)-K(1)	104.34(18)
O(8)-C(33)	1.424(4)	C(27)-O(4)-C(26)	113.0(2)
O(8)-C(32)	1.430(4)	C(27)-O(4)-K(1)	108.34(17)
O(9)-C(34)	1.422(4)	C(26)-O(4)-K(1)	121.32(19)
O(9)-C(35)	1.427(4)	C(29)-O(5)-C(28)	111.9(2)
O(10)-C(37)	1.420(3)	C(29)-O(5)-K(1)	114.50(18)
O(10)-C(36)	1.430(4)	C(28)-O(5)-K(1)	115.66(17)
O(11)-C(39)	1.417(4)	C(40)-O(7)-C(31)	113.2(3)
O(11)-C(38)	1.426(4)	C(40)-O(7)-K(1)	115.06(19)
N(1)-C(3)	1.369(4)	C(31)-O(7)-K(1)	115.95(19)
N(1)-C(2)	1.370(4)	C(33)-O(8)-C(32)	113.5(3)
C(1)-C(2)	1.349(4)	C(33)-O(8)-K(1)	121.83(18)
C(3)-C(4)	1.350(4)	C(32)-O(8)-K(1)	107.13(18)
C(4)-P(2)	1.793(3)	C(34)-O(9)-C(35)	112.3(2)
P(2)-C(5)	1.885(3)	C(34)-O(9)-K(1)	106.35(18)
P(2)-C(9)	1.894(3)	C(35)-O(9)-K(1)	108.46(17)
C(5)-C(7A)	1.507(12)	C(37)-O(10)-C(36)	113.6(2)
C(5)-C(8)	1.513(6)	C(37)-O(10)-K(1)	112.16(17)
C(5)-C(6A)	1.524(12)	C(36)-O(10)-K(1)	119.98(17)
C(5)-C(6)	1.543(6)	C(39)-O(11)-C(38)	114.2(3)

C(5)-C(7)	1.543(6)	C(39)-O(11)-K(1)	110.03(19)
C(5)-C(8A)	1.586(12)	C(38)-O(11)-K(1)	117.15(18)
C(9)-C(11)	1.521(4)	C(3)-N(1)-C(2)	118.3(2)
C(9)-C(10)	1.530(5)	C(3)-N(1)-Ir(1)	120.79(19)
C(9)-C(12)	1.531(5)	C(2)-N(1)-Ir(1)	120.92(19)
C(13)-C(16)	1.525(5)	C(2)-C(1)-P(1)	114.2(2)
C(13)-C(15)	1.526(4)	C(1)-C(2)-N(1)	121.2(3)
C(13)-C(14)	1.532(5)	C(4)-C(3)-N(1)	121.3(3)
C(17)-C(20)	1.526(4)	C(3)-C(4)-P(2)	114.2(2)
C(17)-C(19)	1.529(5)	C(4)-P(2)-C(5)	104.72(15)
C(17)-C(18)	1.529(5)	C(4)-P(2)-C(9)	103.00(15)
C(21)-C(22)	1.513(5)	C(5)-P(2)-C(9)	110.81(15)
C(23)-C(24)	1.484(5)	C(4)-P(2)-Ir(1)	101.51(11)
C(25)-C(26)	1.489(5)	C(5)-P(2)-Ir(1)	116.81(12)
C(27)-C(28)	1.498(4)	C(9)-P(2)-Ir(1)	117.53(11)
C(29)-C(30)	1.499(5)	C(7A)-C(5)-C(6A)	114.7(12)
C(31)-C(32)	1.504(5)	C(8)-C(5)-C(6)	110.8(4)
C(33)-C(34)	1.499(5)	C(8)-C(5)-C(7)	108.2(5)
C(35)-C(36)	1.491(4)	C(6)-C(5)-C(7)	107.9(4)
C(37)-C(38)	1.499(4)	C(7A)-C(5)-C(8A)	107.1(13)
C(39)-C(40)	1.504(5)	C(6A)-C(5)-C(8A)	103.9(12)
N(1)-Ir(1)-P(2)	82.16(7)	C(7A)-C(5)-P(2)	113.2(12)
N(1)-Ir(1)-P(1)	81.86(7)	C(8)-C(5)-P(2)	106.1(4)
P(2)-Ir(1)-P(1)	164.00(3)	C(6A)-C(5)-P(2)	113.9(9)
N(1)-Ir(1)-Cl(1)	178.72(7)	C(6)-C(5)-P(2)	114.4(4)
P(2)-Ir(1)-Cl(1)	98.25(3)	C(7)-C(5)-P(2)	109.1(4)
P(1)-Ir(1)-Cl(1)	97.74(3)	C(8A)-C(5)-P(2)	102.5(11)
O(7)-K(1)-O(4)	158.25(7)	C(11)-C(9)-C(10)	110.3(3)
O(7)-K(1)-O(8)	61.72(7)	C(11)-C(9)-C(12)	108.6(3)
O(4)-K(1)-O(8)	102.10(7)	C(10)-C(9)-C(12)	107.0(3)
O(7)-K(1)-O(1)	84.09(7)	C(11)-C(9)-P(2)	111.0(2)
O(4)-K(1)-O(1)	117.64(7)	C(10)-C(9)-P(2)	115.7(2)
O(8)-K(1)-O(1)	126.62(7)	C(12)-C(9)-P(2)	103.8(2)
O(7)-K(1)-O(5)	136.98(7)	C(16)-C(13)-C(15)	110.5(3)

O(4)-K(1)-O(5)	61.52(6)	C(16)-C(13)-C(14)	108.4(3)
O(8)-K(1)-O(5)	160.22(7)	C(15)-C(13)-C(14)	108.4(3)
O(1)-K(1)-O(5)	60.98(6)	C(16)-C(13)-P(1)	114.8(2)
O(7)-K(1)-O(10)	100.59(7)	C(15)-C(13)-P(1)	110.5(2)
O(4)-K(1)-O(10)	71.79(6)	C(14)-C(13)-P(1)	103.9(2)
O(8)-K(1)-O(10)	114.41(6)	C(20)-C(17)-C(19)	107.6(3)
O(1)-K(1)-O(10)	111.09(7)	C(20)-C(17)-C(18)	107.6(3)
O(5)-K(1)-O(10)	72.80(6)	C(19)-C(17)-C(18)	110.5(3)
O(7)-K(1)-O(2)	76.16(7)	C(20)-C(17)-P(1)	104.0(2)
O(4)-K(1)-O(2)	114.19(7)	C(19)-C(17)-P(1)	114.8(2)
O(8)-K(1)-O(2)	71.64(6)	C(18)-C(17)-P(1)	111.7(2)
O(1)-K(1)-O(2)	60.56(7)	O(1)-C(21)-C(22)	107.3(3)
O(5)-K(1)-O(2)	103.74(7)	O(2)-C(22)-C(21)	112.6(3)
O(10)-K(1)-O(2)	171.08(7)	O(2)-C(23)-C(24)	108.8(3)
O(7)-K(1)-O(11)	60.84(7)	O(3)-C(24)-C(23)	108.4(3)
O(4)-K(1)-O(11)	125.26(7)	O(3)-C(25)-C(26)	107.4(3)
O(8)-K(1)-O(11)	118.73(7)	O(4)-C(26)-C(25)	109.4(3)
O(1)-K(1)-O(11)	65.19(7)	O(4)-C(27)-C(28)	112.8(3)
O(5)-K(1)-O(11)	80.97(6)	O(5)-C(28)-C(27)	109.3(3)
O(10)-K(1)-O(11)	59.26(6)	O(5)-C(29)-C(30)	109.6(3)
O(2)-K(1)-O(11)	112.39(7)	O(1)-C(30)-C(29)	112.0(3)
O(7)-K(1)-O(9)	80.33(6)	O(7)-C(31)-C(32)	109.2(3)
O(4)-K(1)-O(9)	78.43(6)	O(8)-C(32)-C(31)	112.3(3)
O(8)-K(1)-O(9)	56.92(6)	O(8)-C(32)-K(1)	50.11(14)
O(1)-K(1)-O(9)	158.43(6)	C(31)-C(32)-K(1)	83.63(19)
O(5)-K(1)-O(9)	124.16(6)	O(8)-C(33)-C(34)	109.5(3)
O(10)-K(1)-O(9)	57.98(6)	O(9)-C(34)-C(33)	107.7(3)
O(2)-K(1)-O(9)	128.55(6)	O(9)-C(35)-C(36)	108.3(3)
O(11)-K(1)-O(9)	94.05(6)	O(10)-C(36)-C(35)	107.8(3)
O(7)-K(1)-O(3)	126.74(7)	O(10)-C(37)-C(38)	112.1(3)
O(4)-K(1)-O(3)	57.00(6)	O(11)-C(38)-C(37)	107.6(3)
O(8)-K(1)-O(3)	78.61(6)	O(11)-C(39)-C(40)	113.1(3)
O(1)-K(1)-O(3)	93.85(7)	O(7)-C(40)-C(39)	108.0(3)

[Ir(CO){N(CHCHP*t*Bu$_2$)$_2$}] (4)

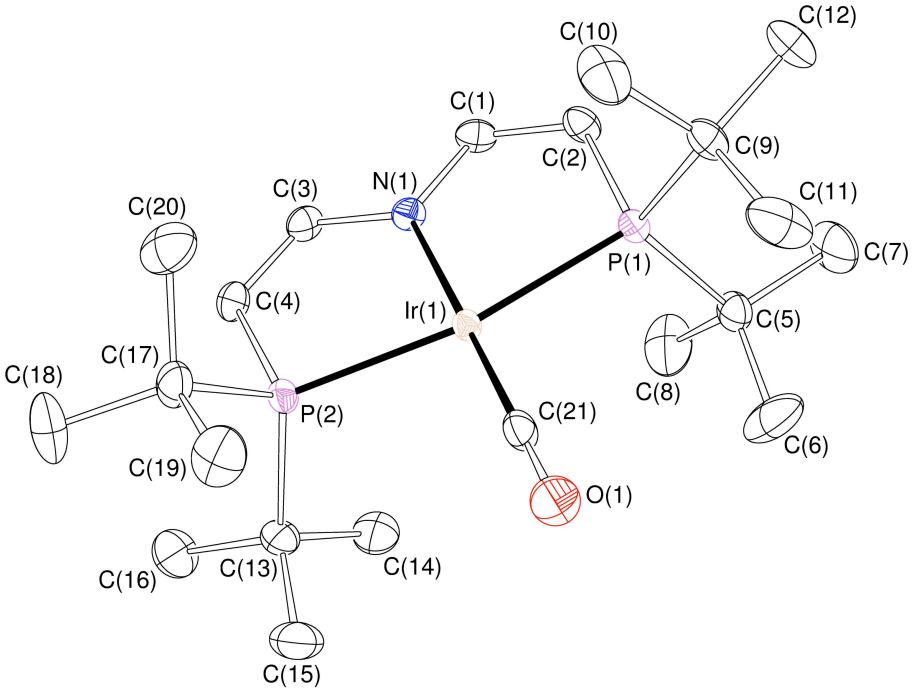

Figure S2. ORTEP plot of **4** with the anisotropic displacement parameters drawn at the 50% probability level. The hydrogen atoms are omitted for clarity.

Table S3. Crystal data and structure refinement for **4**.

CCDC no.	967914	
Empirical formula	$C_{21}H_{40}IrNOP_2$	
Formula weight	576.68 g/mol	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.9010(3) Å	α= 90°
	b = 26.8610(12) Å	β= 106.864(5)°
	c = 11.8140(10) Å	γ = 90°
Volume	2399.4(2) Å^3	
Z	4	
Density (calculated)	1.596 Mg/m^3	
Absorption coefficient	5.708 mm^{-1}	
F(000)	1152	
Crystal size	0.24 x 0.16 x 0.04 mm^3	
Theta range for data collection	3.03 to 28.70°	

Index ranges	-10<=h<=10, -36<=k<=36, -15<=l<=15
Reflections collected	69417
Independent reflections	6192 [R(int) = 0.0524]
Completeness to theta = 28.70°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0 and 0.612
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6192 / 0 / 247
Goodness-of-fit on F^2	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0199, wR2 = 0.0400
R indices (all data)	R1 = 0.0248, wR2 = 0.0413
Largest diff. peak and hole	0.916 and -0.810 eÅ^{-3}

Table S4. Bond lengths [Å] and angles [°] for **4**.

Ir(1)-C(21)	1.829(2)	C(4)-P(2)-C(17)	105.34(12)
Ir(1)-N(1)	2.0608(19)	C(4)-P(2)-C(13)	105.38(12)
Ir(1)-P(2)	2.3080(6)	C(17)-P(2)-C(13)	112.91(12)
Ir(1)-P(1)	2.3137(6)	C(4)-P(2)-Ir(1)	100.99(8)
P(1)-C(2)	1.790(2)	C(17)-P(2)-Ir(1)	116.51(9)
P(1)-C(9)	1.873(2)	C(13)-P(2)-Ir(1)	113.86(8)
P(1)-C(5)	1.882(3)	C(1)-N(1)-C(3)	120.4(2)
P(2)-C(4)	1.791(2)	C(1)-N(1)-Ir(1)	119.94(15)
P(2)-C(17)	1.874(3)	C(3)-N(1)-Ir(1)	119.71(16)
P(2)-C(13)	1.884(3)	C(2)-C(1)-N(1)	122.4(2)
N(1)-C(1)	1.367(3)	C(1)-C(2)-P(1)	114.76(18)
N(1)-C(3)	1.371(3)	C(4)-C(3)-N(1)	122.3(2)
O(1)-C(21)	1.153(3)	C(3)-C(4)-P(2)	114.93(18)
C(1)-C(2)	1.347(3)	C(6)-C(5)-C(7)	110.0(2)
C(3)-C(4)	1.351(3)	C(6)-C(5)-C(8)	108.3(3)
C(5)-C(6)	1.527(4)	C(7)-C(5)-C(8)	108.4(3)
C(5)-C(7)	1.528(4)	C(6)-C(5)-P(1)	110.68(19)
C(5)-C(8)	1.533(4)	C(7)-C(5)-P(1)	113.98(19)
C(9)-C(10)	1.526(4)	C(8)-C(5)-P(1)	105.26(18)
C(9)-C(11)	1.528(4)	C(10)-C(9)-C(11)	109.6(3)

C(9)-C(12)	1.529(3)	C(10)-C(9)-C(12)	108.1(2)
C(13)-C(14)	1.530(4)	C(11)-C(9)-C(12)	109.3(2)
C(13)-C(15)	1.530(4)	C(10)-C(9)-P(1)	104.83(18)
C(13)-C(16)	1.543(4)	C(11)-C(9)-P(1)	111.08(18)
C(17)-C(20)	1.528(4)	C(12)-C(9)-P(1)	113.77(18)
C(17)-C(19)	1.531(4)	C(14)-C(13)-C(15)	108.6(2)
C(17)-C(18)	1.532(4)	C(14)-C(13)-C(16)	107.8(2)
C(21)-Ir(1)-N(1)	178.20(9)	C(15)-C(13)-C(16)	110.2(2)
C(21)-Ir(1)-P(2)	97.42(7)	C(14)-C(13)-P(2)	105.53(17)
N(1)-Ir(1)-P(2)	82.11(6)	C(15)-C(13)-P(2)	111.76(19)
C(21)-Ir(1)-P(1)	98.88(7)	C(16)-C(13)-P(2)	112.72(19)
N(1)-Ir(1)-P(1)	81.70(6)	C(20)-C(17)-C(19)	108.2(2)
P(2)-Ir(1)-P(1)	163.37(2)	C(20)-C(17)-C(18)	109.1(2)
C(2)-P(1)-C(9)	105.52(11)	C(19)-C(17)-C(18)	109.6(2)
C(2)-P(1)-C(5)	105.87(12)	C(20)-C(17)-P(2)	105.62(18)
C(9)-P(1)-C(5)	112.94(12)	C(19)-C(17)-P(2)	110.70(18)
C(2)-P(1)-Ir(1)	101.00(8)	C(18)-C(17)-P(2)	113.4(2)
C(9)-P(1)-Ir(1)	116.65(8)	O(1)-C(21)-Ir(1)	178.7(2)
C(5)-P(1)-Ir(1)	113.16(8)		

[Ir(H)(C_6H_5){N(CHCHP*t*Bu_2)$_2$}] (5)

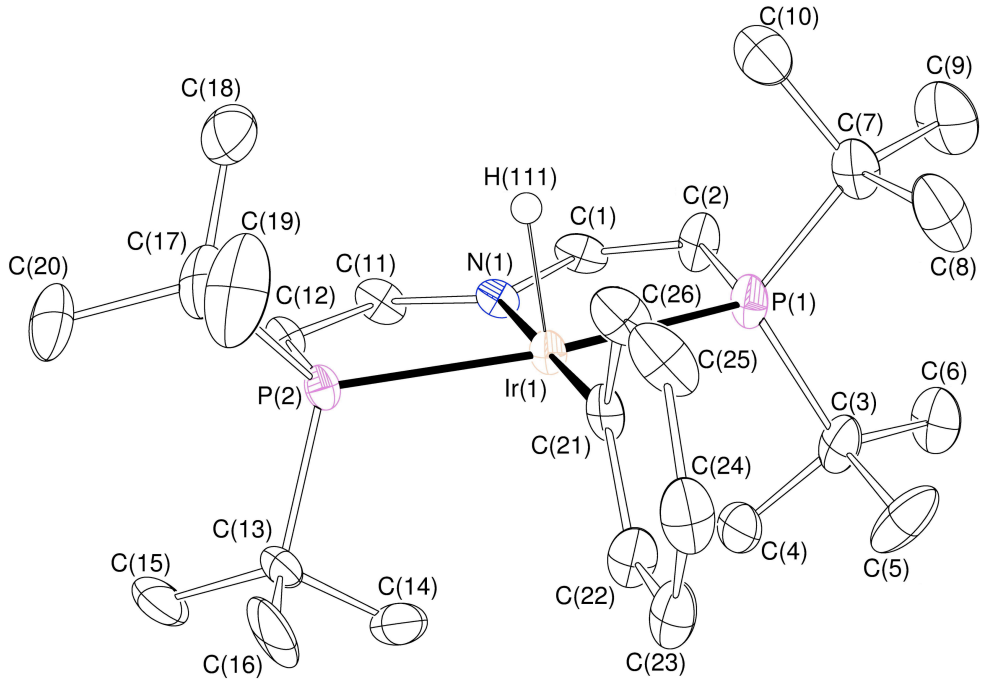

Figure S3. ORTEP plot of **5** with the anisotropic displacement parameters drawn at the 50% probability level. The hydrogen atoms are omitted for clarity.

Table S5. Crystal data and structure refinement for **5**.

CCDC no.	967915	
Empirical formula	$C_{26}H_{46}IrNP_2$	
Formula weight	626.78 g/mol	
Temperature	100(2) K	
Wavelength	0.56086 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.896(2) Å	α = 90°
	b = 29.428(7) Å	β = 100.058(5)°
	c = 10.601(2) Å	γ = 90°
Volume	2732.5(11) $Å^3$	
Z	4	
Density (calculated)	1.524 Mg/m^3	
Absorption coefficient	2.729 mm^{-1}	
F(000)	1264	
Crystal size	0.110 x 0.070 x 0.060 mm^3	

Theta range for data collection	1.634 to 20.554°	
Index ranges	-11<=h<=11, -36<=k<=36, -13<=l<=13	
Reflections collected	24583	
Independent reflections	5543 [R(int) = 0.0561]	
Completeness to theta = 19.665°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5599 and 0.4793	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5543 / 89 / 287	
Goodness-of-fit on F^2	1.134	
Final R indices [I>2sigma(I)]	R1 = 0.0494,	wR2 = 0.1477
R indices (all data)	R1 = 0.0615,	wR2 = 0.1545
Largest diff. peak and hole	1.428 and -3.398 eÅ^{-3}	

Table S6. Bond lengths [Å] and angles [°] for **5**.

C(1)-N(1)	1.348(10)	C(9)-C(7)-P(1)	111.7(7)
C(1)-C(2)	1.362(12)	C(12)-C(11)-N(1)	122.2(7)
C(2)-P(1)	1.786(8)	C(11)-C(12)-P(2)	115.8(6)
C(3)-C(5)	1.530(12)	C(16)-C(13)-C(14)	108.0(8)
C(3)-C(6)	1.549(11)	C(16)-C(13)-C(15)	111.1(8)
C(3)-C(4)	1.581(14)	C(14)-C(13)-C(15)	107.4(9)
C(3)-P(1)	1.870(9)	C(16)-C(13)-P(2)	111.2(7)
C(7)-C(8)	1.535(11)	C(14)-C(13)-P(2)	103.3(6)
C(7)-C(10)	1.535(14)	C(15)-C(13)-P(2)	115.1(6)
C(7)-C(9)	1.559(11)	C(19)-C(17)-C(20)	110.4(8)
C(7)-P(1)	1.886(9)	C(19)-C(17)-C(18)	109.0(9)
C(11)-C(12)	1.352(10)	C(20)-C(17)-C(18)	109.9(8)
C(11)-N(1)	1.357(10)	C(19)-C(17)-P(2)	110.9(7)
C(12)-P(2)	1.792(7)	C(20)-C(17)-P(2)	111.5(6)
C(13)-C(16)	1.532(14)	C(18)-C(17)-P(2)	104.9(6)
C(13)-C(14)	1.535(14)	C(26)-C(21)-C(22)	114.7(7)
C(13)-C(15)	1.547(12)	C(26)-C(21)-Ir(1)	123.1(6)
C(13)-P(2)	1.864(9)	C(22)-C(21)-Ir(1)	122.2(6)
C(17)-C(19)	1.526(13)	C(23)-C(22)-C(21)	122.6(8)

C(17)-C(20)	1.545(13)	C(24)-C(23)-C(22)	120.2(8)
C(17)-C(18)	1.559(14)	C(25)-C(24)-C(23)	118.7(8)
C(17)-P(2)	1.887(9)	C(24)-C(25)-C(26)	120.7(8)
C(21)-C(26)	1.393(12)	C(21)-C(26)-C(25)	123.1(8)
C(21)-C(22)	1.413(11)	C(1)-N(1)-C(11)	120.3(7)
C(21)-Ir(1)	2.080(7)	C(1)-N(1)-Ir(1)	119.6(5)
C(22)-C(23)	1.405(11)	C(11)-N(1)-Ir(1)	119.7(5)
C(23)-C(24)	1.386(12)	C(2)-P(1)-C(3)	104.0(4)
C(24)-C(25)	1.371(13)	C(2)-P(1)-C(7)	105.2(4)
C(25)-C(26)	1.401(11)	C(3)-P(1)-C(7)	112.7(4)
N(1)-Ir(1)	2.109(6)	C(2)-P(1)-Ir(1)	100.3(3)
P(1)-Ir(1)	2.337(2)	C(3)-P(1)-Ir(1)	112.5(3)
P(2)-Ir(1)	2.3276(19)	C(7)-P(1)-Ir(1)	119.7(3)
N(1)-C(1)-C(2)	121.9(7)	C(12)-P(2)-C(13)	104.7(4)
C(1)-C(2)-P(1)	116.3(6)	C(12)-P(2)-C(17)	103.9(4)
C(5)-C(3)-C(6)	109.1(7)	C(13)-P(2)-C(17)	112.7(5)
C(5)-C(3)-C(4)	108.9(8)	C(12)-P(2)-Ir(1)	101.0(2)
C(6)-C(3)-C(4)	106.0(8)	C(13)-P(2)-Ir(1)	111.6(3)
C(5)-C(3)-P(1)	112.6(6)	C(17)-P(2)-Ir(1)	120.6(3)
C(6)-C(3)-P(1)	115.7(6)	C(21)-Ir(1)-N(1)	179.8(3)
C(4)-C(3)-P(1)	104.1(6)	C(21)-Ir(1)-P(2)	98.7(2)
C(8)-C(7)-C(10)	108.8(8)	N(1)-Ir(1)-P(2)	81.26(18)
C(8)-C(7)-C(9)	109.4(8)	C(21)-Ir(1)-P(1)	98.7(2)
C(10)-C(7)-C(9)	108.2(8)	N(1)-Ir(1)-P(1)	81.33(18)
C(8)-C(7)-P(1)	112.3(6)	P(2)-Ir(1)-P(1)	162.58(7)
C(10)-C(7)-P(1)	106.3(6)		

[Ir(O$_2$){N(CHCHP*t*Bu$_2$)$_2$}] (8)

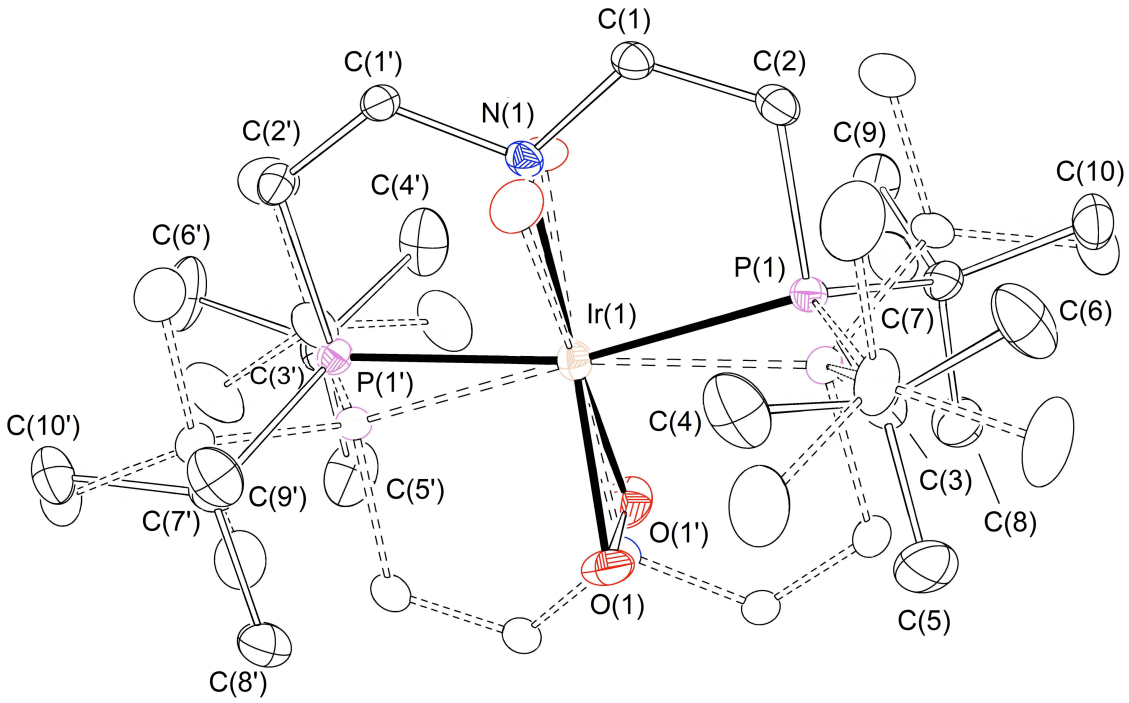

Figure S4. ORTEP plot of **8** with the anisotropic displacement parameters drawn at the 50% probability level. The hydrogen atoms are omitted for clarity.

Table S7. Crystal data and structure refinement for **8**.

CCDC no.	973313	
Empirical formula	$C_{20}H_{40}IrNO_2P_2$	
Formula weight	580.67	
Temperature	100(2) K	
Wavelength	0.56086 Å	
Crystal system	Monoclinic	
Space group	C2/m	
Unit cell dimensions	a = 13.917(3) Å	α= 90°
	b = 7.7210(15) Å	β= 111.39(3)°
	c = 11.629(2) Å	γ = 90°
Volume	1163.5(5) Å3	
Z	2	
Density (calculated)	1.657 Mg/m^3	
Absorption coefficient	3.203 mm^{-1}	
F(000)	580	

Crystal size	0.090 x 0.080 x 0.060 mm^3	
Theta range for data collection	2.381 to 23.612°	
Index ranges	-19<=h<=19, -11<=k<=11, -16<=l<=16	
Reflections collected	19582	
Independent reflections	1891 [R(int) = 0.0592]	
Completeness to theta = 19.665°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7459 and 0.6594	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1891 / 161 / 126	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0168,	wR2 = 0.0370
R indices (all data)	R1 = 0.0168,	wR2 = 0.0370
Largest diff. peak and hole	1.260 and -0.743 $eÅ^{-3}$	

Table S8. Bond lengths [Å] and angles [°] for **8**.

Ir(1)-O(1)	1.945(3)	C(2)-P(1)-C(3)	104.2(4)
Ir(1)-N(1)	2.015(5)	C(7)-P(1)-C(3)	113.9(2)
Ir(1)-P(1)	2.3461(13)	C(2)-P(1)-Ir(1)	101.16(12)
P(1)-C(2)	1.794(4)	C(7)-P(1)-Ir(1)	116.05(11)
P(1)-C(7)	1.866(3)	C(3)-P(1)-Ir(1)	113.40(14)
P(1)-C(3)	1.873(4)	C(6)-C(3)-C(5)	109.7(5)
C(3)-C(6)	1.534(6)	C(6)-C(3)-C(4)	108.7(6)
C(3)-C(5)	1.536(12)	C(5)-C(3)-C(4)	109.2(5)
C(3)-C(4)	1.537(6)	C(6)-C(3)-P(1)	113.6(4)
C(7)-C(10)	1.536(7)	C(5)-C(3)-P(1)	110.5(5)
C(7)-C(9)	1.536(5)	C(4)-C(3)-P(1)	104.9(4)
C(7)-C(8)	1.537(5)	C(10)-C(7)-C(9)	108.5(5)
N(1)-C(1)	1.407(4)	C(10)-C(7)-C(8)	110.2(8)
O(1)-O(1')	1.415(7)	C(9)-C(7)-C(8)	108.0(3)
C(1)-C(2)	1.352(5)	C(10)-C(7)-P(1)	113.9(4)
O(1)-Ir(1)-O(1')	42.7(2)	C(9)-C(7)-P(1)	105.4(2)
O(1)-Ir(1)-N(1)	158.66(11)	C(8)-C(7)-P(1)	110.4(3)
O(1)-Ir(1)-P(1)	96.11(10)	C(1)-N(1)-Ir(1)	121.8(2)

O(1')-Ir(1)-P(1)	99.93(10)	O(1')-O(1)-Ir(1)	68.66(11)
N(1)-Ir(1)-P(1)	81.40(2)	C(2)-C(1)-N(1)	121.2(3)
P(1)-Ir(1)-P(1')	162.79(4)	C(1)-C(2)-P(1)	114.4(3)
C(2)-P(1)-C(7)	106.16(15)		