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Iridium Complexes Bearing a PNP Ligand, Favoring Facile C(sp^3)-H Bond Cleavage

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A. General Considerations for X-Ray Crystallography

Diffraction data for the complexes were collected at low temperature (T = 100 K) on a Bruker SMART APEX CCD diffractometer with graphite-monochromated Mo Kα radiation (λ= 0.71073 Å). The cell parameters for the Ir complexes were obtained from the least-squares refinement of the spots (from 60 collected frames) using the SMART program. A hemisphere of the crystal data was collected and the intensity data was processed using the Saint Plus program. All calculations for structure determination were carried out using the SHELXTL package (version 5.1). 2 Initial atomic positions were located by direct methods using XS, and the structure was refined by least-squares methods using SHELX. Absorption corrections were applied by using SADABS.3 Calculated hydrogen positions were input and refined in a riding manner along with the attached carbons.[1]

B. X-Ray Diffraction Data for Ir(PNP)(Cl)$_3$ (2).

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Table 1. Crystal data and structure refinement for C46 H86 Cl6 Ir2 N2 P4 * C1 H2 Cl2.

Identification code	perianam	
Empirical formula	C47 H88 Cl8 Ir2 N2 P4	
Formula weight	1473.07	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.2633(14) Å	α= 106.729(2)°.
	b = 14.7326(16) Å	β= 95.934(2)°.
	c = 17.4332(18) Å	γ = 112.653(2)°.
Volume	2920.8(5) $Å^3$	
Z	2	
Density (calculated)	1.675 Mg/m^3	
Absorption coefficient	5.060 mm^{-1}	
F(000)	1468	
Crystal size	0.16 x 0.05 x 0.02 mm^3	
Theta range for data collection	1.26 to 28.34°.	
Index ranges	-17<=h<=16, -19<=k<=19, -16<=l<=22	
Reflections collected	19155	
Independent reflections	13373 [R(int) = 0.0254]	
Completeness to theta = 28.34°	91.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.745 and 0.581	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13373 / 6 / 592	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1169	
R indices (all data)	R1 = 0.0544, wR2 = 0.1283	
Largest diff. peak and hole	4.786 and -1.897 $e.Å^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for C46 H86 Cl6 Ir2 N2 P4 * C1 H2 Cl2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	6403(1)	3407(1)	3431(1)	14(1)
Cl(1)	4757(1)	3673(1)	3459(1)	20(1)
Cl(2)	5320(1)	1553(1)	2854(1)	21(1)
Cl(3)	8100(1)	3224(1)	3449(1)	19(1)
P(1)	6570(1)	3634(1)	4869(1)	15(1)
P(2)	6494(1)	3678(1)	2155(1)	17(1)
N(1)	7307(4)	5014(4)	3898(3)	16(1)
C(1)	7945(5)	3925(5)	5573(4)	19(1)
C(2)	8883(5)	4879(5)	5490(4)	23(1)
C(3)	7937(6)	4228(5)	6481(4)	23(1)
C(4)	8256(5)	3002(5)	5327(4)	23(1)
C(5)	5367(5)	2818(5)	5233(4)	21(1)
C(6)	5561(6)	1894(5)	5332(4)	25(1)
C(7)	5223(5)	3479(5)	6039(4)	25(1)
C(8)	4237(6)	2319(6)	4591(4)	32(2)
C(9)	6615(5)	4970(4)	5149(3)	17(1)
C(10)	7294(5)	5570(5)	4661(4)	18(1)
C(11)	7862(5)	6647(5)	4977(4)	23(1)
C(12)	8485(5)	7172(5)	4518(4)	22(1)
C(13)	8500(5)	6594(5)	3741(4)	22(1)
C(14)	7902(5)	5494(5)	3439(4)	18(1)
C(15)	7862(5)	4850(4)	2582(3)	18(1)
C(16)	6666(5)	2725(5)	1244(3)	22(1)
C(17)	7214(6)	2071(5)	1530(4)	28(1)
C(18)	7432(6)	3315(6)	761(4)	30(2)
C(19)	5504(6)	1911(5)	690(4)	28(1)
C(20)	5516(5)	4170(5)	1734(4)	19(1)
C(21)	5686(5)	5207(5)	2405(4)	23(1)
C(22)	5766(6)	4460(5)	981(4)	25(1)
C(23)	4280(5)	3346(5)	1517(4)	23(1)
Ir(2)	9414(1)	8953(1)	2170(1)	14(1)

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Cl(4)	8711(1)	8733(1)	794(1)	20(1)
Cl(5)	8542(1)	7094(1)	1816(1)	21(1)
Cl(6)	10119(1)	9229(1)	3567(1)	20(1)
P(3)	11207(1)	9097(1)	1931(1)	16(1)
P(4)	7865(1)	9324(1)	2492(1)	16(1)
N(2)	10183(4)	10547(4)	2438(3)	17(1)
C(24)	11871(5)	8283(5)	2242(4)	23(1)
C(25)	11400(6)	7900(6)	2893(4)	27(1)
C(26)	11632(6)	7317(5)	1489(4)	31(2)
C(27)	13160(5)	8927(5)	2620(4)	28(1)
C(28)	11583(5)	9283(5)	946(4)	19(1)
C(29)	10843(6)	8320(5)	183(4)	30(2)
C(30)	12831(5)	9546(5)	952(4)	25(1)
C(31)	11411(5)	10225(5)	858(4)	24(1)
C(32)	11975(5)	10439(5)	2696(3)	19(1)
C(33)	11319(5)	11059(5)	2648(3)	20(1)
C(34)	11851(5)	12119(5)	2772(4)	24(1)
C(35)	11211(6)	12666(5)	2685(4)	26(1)
C(36)	10055(6)	12137(5)	2503(4)	27(1)
C(37)	9544(5)	11069(5)	2367(3)	19(1)
C(38)	8281(5)	10470(4)	2158(4)	19(1)
C(39)	6352(5)	8418(4)	1892(3)	17(1)
C(40)	6284(5)	7645(5)	1062(4)	25(1)
C(41)	5731(5)	9046(5)	1713(4)	26(1)
C(42)	5761(5)	7763(5)	2381(4)	24(1)
C(43)	7859(5)	9928(5)	3610(4)	20(1)
C(44)	7755(5)	9167(5)	4064(4)	24(1)
C(45)	6936(5)	10295(5)	3722(4)	23(1)
C(46)	8995(5)	10929(5)	4037(4)	24(1)
C(47)	8166(7)	5954(7)	9527(6)	54(2)
Cl(7)	8931(3)	5768(2)	8778(2)	94(1)
Cl(8)	6858(2)	4816(2)	9231(1)	49(1)

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Table 3. Bond lengths [Å] and angles [°] for C46 H86 Cl6 Ir2 N2 P4 * C1 H2 Cl2.

Ir(1)-N(1)	2.052(5)
Ir(1)-Cl(1)	2.3643(14)
Ir(1)-Cl(3)	2.3666(14)
Ir(1)-Cl(2)	2.3735(14)
Ir(1)-P(2)	2.3775(15)
Ir(1)-P(1)	2.4049(15)
P(1)-C(9)	1.862(6)
P(1)-C(5)	1.889(6)
P(1)-C(1)	1.910(6)
P(2)-C(15)	1.842(6)
P(2)-C(16)	1.893(6)
P(2)-C(20)	1.893(6)
N(1)-C(14)	1.337(7)
N(1)-C(10)	1.353(7)
C(1)-C(3)	1.519(8)
C(1)-C(4)	1.528(8)
C(1)-C(2)	1.534(8)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.531(9)
C(5)-C(8)	1.539(9)
C(5)-C(7)	1.540(8)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800

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C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.513(8)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.371(8)
C(11)-C(12)	1.387(8)
C(11)-H(11)	0.9500
C(12)-C(13)	1.383(8)
C(12)-H(12)	0.9500
C(13)-C(14)	1.402(8)
C(13)-H(13)	0.9500
C(14)-C(15)	1.505(8)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(19)	1.532(9)
C(16)-C(18)	1.554(9)
C(16)-C(17)	1.564(8)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(22)	1.523(8)
C(20)-C(23)	1.542(8)
C(20)-C(21)	1.550(8)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800

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C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
Ir(2)-N(2)	2.049(5)
Ir(2)-Cl(4)	2.3640(14)
Ir(2)-Cl(6)	2.3744(14)
Ir(2)-Cl(5)	2.3781(14)
Ir(2)-P(3)	2.3971(15)
Ir(2)-P(4)	2.3995(15)
P(3)-C(32)	1.838(6)
P(3)-C(24)	1.896(6)
P(3)-C(28)	1.901(6)
P(4)-C(38)	1.847(6)
P(4)-C(39)	1.897(6)
P(4)-C(43)	1.899(6)
N(2)-C(33)	1.351(8)
N(2)-C(37)	1.364(7)
C(24)-C(25)	1.497(9)
C(24)-C(26)	1.530(9)
C(24)-C(27)	1.554(9)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.522(8)
C(28)-C(31)	1.537(8)
C(28)-C(30)	1.546(8)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800

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C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(33)	1.496(8)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.382(9)
C(34)-C(35)	1.400(9)
C(34)-H(34)	0.9500
C(35)-C(36)	1.377(9)
C(35)-H(35)	0.9500
C(36)-C(37)	1.387(9)
C(36)-H(36)	0.9500
C(37)-C(38)	1.506(8)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(42)	1.517(8)
C(39)-C(41)	1.527(8)
C(39)-C(40)	1.531(8)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(44)	1.522(9)
C(43)-C(45)	1.525(8)
C(43)-C(46)	1.556(8)
C(44)-H(44A)	0.9800

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C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-Cl(7)	1.759(9)
C(47)-Cl(8)	1.778(8)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900

N(1)-Ir(1)-Cl(1)	87.50(13)
N(1)-Ir(1)-Cl(3)	89.91(13)
Cl(1)-Ir(1)-Cl(3)	177.26(5)
N(1)-Ir(1)-Cl(2)	178.06(14)
Cl(1)-Ir(1)-Cl(2)	91.36(5)
Cl(3)-Ir(1)-Cl(2)	91.26(5)
N(1)-Ir(1)-P(2)	82.04(14)
Cl(1)-Ir(1)-P(2)	91.56(5)
Cl(3)-Ir(1)-P(2)	88.95(5)
Cl(2)-Ir(1)-P(2)	96.42(5)
N(1)-Ir(1)-P(1)	82.72(14)
Cl(1)-Ir(1)-P(1)	87.06(5)
Cl(3)-Ir(1)-P(1)	91.74(5)
Cl(2)-Ir(1)-P(1)	98.80(5)
P(2)-Ir(1)-P(1)	164.74(5)
C(9)-P(1)-C(5)	107.0(3)
C(9)-P(1)-C(1)	101.3(3)
C(5)-P(1)-C(1)	107.9(3)
C(9)-P(1)-Ir(1)	92.92(18)
C(5)-P(1)-Ir(1)	121.12(19)
C(1)-P(1)-Ir(1)	121.88(19)
C(15)-P(2)-C(16)	106.5(3)
C(15)-P(2)-C(20)	104.0(3)

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C(16)-P(2)-C(20)	107.4(3)
C(15)-P(2)-Ir(1)	94.25(19)
C(16)-P(2)-Ir(1)	122.0(2)
C(20)-P(2)-Ir(1)	119.2(2)
C(14)-N(1)-C(10)	121.1(5)
C(14)-N(1)-Ir(1)	119.2(4)
C(10)-N(1)-Ir(1)	119.7(4)
C(3)-C(1)-C(4)	109.1(5)
C(3)-C(1)-C(2)	106.2(5)
C(4)-C(1)-C(2)	108.1(5)
C(3)-C(1)-P(1)	113.5(4)
C(4)-C(1)-P(1)	112.0(4)
C(2)-C(1)-P(1)	107.7(4)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(1)-C(3)-H(3A)	109.5
C(1)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(1)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(8)	105.7(5)
C(6)-C(5)-C(7)	111.5(5)
C(8)-C(5)-C(7)	106.9(5)
C(6)-C(5)-P(1)	108.9(4)
C(8)-C(5)-P(1)	111.8(4)

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C(7)-C(5)-P(1)	112.0(4)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-P(1)	110.6(4)
C(10)-C(9)-H(9A)	109.5
P(1)-C(9)-H(9A)	109.5
C(10)-C(9)-H(9B)	109.5
P(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	108.1
N(1)-C(10)-C(11)	120.8(5)
N(1)-C(10)-C(9)	118.2(5)
C(11)-C(10)-C(9)	121.0(5)
C(10)-C(11)-C(12)	119.6(6)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(13)-C(12)-C(11)	119.0(6)
C(13)-C(12)-H(12)	120.5
C(11)-C(12)-H(12)	120.5
C(12)-C(13)-C(14)	119.6(6)
C(12)-C(13)-H(13)	120.2

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C(14)-C(13)-H(13)	120.2
N(1)-C(14)-C(13)	119.8(5)
N(1)-C(14)-C(15)	119.4(5)
C(13)-C(14)-C(15)	120.7(5)
C(14)-C(15)-P(2)	109.3(4)
C(14)-C(15)-H(15A)	109.8
P(2)-C(15)-H(15A)	109.8
C(14)-C(15)-H(15B)	109.8
P(2)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.3
C(19)-C(16)-C(18)	112.0(5)
C(19)-C(16)-C(17)	105.1(5)
C(18)-C(16)-C(17)	107.5(5)
C(19)-C(16)-P(2)	109.5(4)
C(18)-C(16)-P(2)	111.3(5)
C(17)-C(16)-P(2)	111.3(4)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(22)-C(20)-C(23)	109.0(5)
C(22)-C(20)-C(21)	105.2(5)

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C(23)-C(20)-C(21)	109.9(5)
C(22)-C(20)-P(2)	114.1(4)
C(23)-C(20)-P(2)	110.5(4)
C(21)-C(20)-P(2)	108.0(4)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(20)-C(23)-H(23A)	109.5
C(20)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(20)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(2)-Ir(2)-Cl(4)	88.80(14)
N(2)-Ir(2)-Cl(6)	89.57(14)
Cl(4)-Ir(2)-Cl(6)	178.13(5)
N(2)-Ir(2)-Cl(5)	178.00(14)
Cl(4)-Ir(2)-Cl(5)	89.72(5)
Cl(6)-Ir(2)-Cl(5)	91.93(5)
N(2)-Ir(2)-P(3)	82.07(14)
Cl(4)-Ir(2)-P(3)	92.57(5)
Cl(6)-Ir(2)-P(3)	88.11(5)
Cl(5)-Ir(2)-P(3)	96.65(5)
N(2)-Ir(2)-P(4)	82.05(14)
Cl(4)-Ir(2)-P(4)	86.88(5)
Cl(6)-Ir(2)-P(4)	91.98(5)
Cl(5)-Ir(2)-P(4)	99.22(5)

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P(3)-Ir(2)-P(4)	164.12(5)
C(32)-P(3)-C(24)	106.3(3)
C(32)-P(3)-C(28)	102.3(3)
C(24)-P(3)-C(28)	109.3(3)
C(32)-P(3)-Ir(2)	93.41(19)
C(24)-P(3)-Ir(2)	121.4(2)
C(28)-P(3)-Ir(2)	119.57(19)
C(38)-P(4)-C(39)	105.5(3)
C(38)-P(4)-C(43)	102.0(3)
C(39)-P(4)-C(43)	107.9(3)
C(38)-P(4)-Ir(2)	94.49(19)
C(39)-P(4)-Ir(2)	122.53(19)
C(43)-P(4)-Ir(2)	119.81(19)
C(33)-N(2)-C(37)	120.8(5)
C(33)-N(2)-Ir(2)	119.4(4)
C(37)-N(2)-Ir(2)	119.7(4)
C(25)-C(24)-C(26)	107.7(5)
C(25)-C(24)-C(27)	105.3(5)
C(26)-C(24)-C(27)	110.3(5)
C(25)-C(24)-P(3)	111.8(4)
C(26)-C(24)-P(3)	109.3(4)
C(27)-C(24)-P(3)	112.2(4)
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-H(27A)	109.5
C(24)-C(27)-H(27B)	109.5

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H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(29)-C(28)-C(31)	107.9(5)
C(29)-C(28)-C(30)	108.7(5)
C(31)-C(28)-C(30)	105.9(5)
C(29)-C(28)-P(3)	111.9(4)
C(31)-C(28)-P(3)	109.1(4)
C(30)-C(28)-P(3)	113.0(4)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(28)-C(31)-H(31A)	109.5
C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(33)-C(32)-P(3)	109.9(4)
C(33)-C(32)-H(32A)	109.7
P(3)-C(32)-H(32A)	109.7
C(33)-C(32)-H(32B)	109.7
P(3)-C(32)-H(32B)	109.7
H(32A)-C(32)-H(32B)	108.2
N(2)-C(33)-C(34)	120.1(5)
N(2)-C(33)-C(32)	118.4(5)

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C(34)-C(33)-C(32)	121.4(5)
C(33)-C(34)-C(35)	120.0(6)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(36)-C(35)-C(34)	118.9(6)
C(36)-C(35)-H(35)	120.6
C(34)-C(35)-H(35)	120.6
C(35)-C(36)-C(37)	119.8(6)
C(35)-C(36)-H(36)	120.1
C(37)-C(36)-H(36)	120.1
N(2)-C(37)-C(36)	120.3(6)
N(2)-C(37)-C(38)	118.8(5)
C(36)-C(37)-C(38)	120.9(5)
C(37)-C(38)-P(4)	110.5(4)
C(37)-C(38)-H(38A)	109.5
P(4)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
P(4)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	108.1
C(42)-C(39)-C(41)	110.4(5)
C(42)-C(39)-C(40)	106.8(5)
C(41)-C(39)-C(40)	107.5(5)
C(42)-C(39)-P(4)	109.3(4)
C(41)-C(39)-P(4)	111.1(4)
C(40)-C(39)-P(4)	111.8(4)
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-H(41A)	109.5
C(39)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(39)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5

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H(41B)-C(41)-H(41C)	109.5
C(39)-C(42)-H(42A)	109.5
C(39)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(39)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(44)-C(43)-C(45)	108.6(5)
C(44)-C(43)-C(46)	108.5(5)
C(45)-C(43)-C(46)	106.1(5)
C(44)-C(43)-P(4)	111.2(4)
C(45)-C(43)-P(4)	114.1(4)
C(46)-C(43)-P(4)	108.1(4)
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(43)-C(46)-H(46A)	109.5
C(43)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(43)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
Cl(7)-C(47)-Cl(8)	108.8(4)
Cl(7)-C(47)-H(47A)	109.9
Cl(8)-C(47)-H(47A)	109.9
Cl(7)-C(47)-H(47B)	109.9
Cl(8)-C(47)-H(47B)	109.9

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H(47A)-C(47)-H(47B)	108.3

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C46 H86 Cl6 Ir2 N2 P4 * C1 H2 Cl2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	12(1)	13(1)	16(1)	5(1)	6(1)	4(1)
Cl(1)	14(1)	24(1)	24(1)	10(1)	8(1)	8(1)
Cl(2)	20(1)	13(1)	24(1)	4(1)	5(1)	3(1)
Cl(3)	16(1)	25(1)	19(1)	8(1)	8(1)	11(1)
P(1)	15(1)	14(1)	16(1)	6(1)	8(1)	5(1)
P(2)	17(1)	17(1)	17(1)	7(1)	6(1)	6(1)
N(1)	9(2)	18(2)	18(2)	5(2)	4(2)	4(2)
C(1)	18(3)	17(3)	20(3)	5(2)	2(2)	7(2)
C(2)	11(3)	27(3)	24(3)	6(2)	4(2)	4(2)
C(3)	29(3)	18(3)	24(3)	9(2)	5(3)	9(3)
C(4)	23(3)	30(3)	20(3)	9(2)	8(2)	15(3)
C(5)	20(3)	21(3)	17(3)	5(2)	9(2)	5(2)
C(6)	29(3)	17(3)	28(3)	7(2)	15(3)	7(3)
C(7)	27(3)	20(3)	29(3)	11(3)	20(3)	9(3)
C(8)	22(3)	46(4)	25(3)	16(3)	13(3)	9(3)
C(9)	16(3)	11(3)	20(3)	6(2)	5(2)	3(2)
C(10)	17(3)	18(3)	21(3)	9(2)	6(2)	7(2)
C(11)	21(3)	24(3)	18(3)	5(2)	5(2)	8(3)
C(12)	15(3)	18(3)	23(3)	6(2)	0(2)	0(2)
C(13)	18(3)	18(3)	23(3)	10(2)	5(2)	-2(2)
C(14)	11(3)	18(3)	21(3)	9(2)	5(2)	2(2)
C(15)	14(3)	16(3)	22(3)	9(2)	7(2)	2(2)
C(16)	28(3)	30(3)	13(3)	6(2)	10(2)	19(3)
C(17)	39(4)	35(4)	20(3)	9(3)	11(3)	27(3)
C(18)	28(4)	40(4)	25(3)	13(3)	15(3)	14(3)
C(19)	34(4)	23(3)	23(3)	2(3)	8(3)	11(3)
C(20)	17(3)	18(3)	23(3)	8(2)	3(2)	8(2)
C(21)	20(3)	29(3)	21(3)	4(2)	4(2)	16(3)
C(22)	29(3)	32(4)	16(3)	7(3)	7(2)	15(3)
C(23)	20(3)	19(3)	30(3)	10(2)	8(2)	7(2)

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Ir(2)	14(1)	13(1)	15(1)	6(1)	6(1)	5(1)
Cl(4)	21(1)	21(1)	18(1)	9(1)	6(1)	7(1)
Cl(5)	23(1)	14(1)	25(1)	9(1)	9(1)	5(1)
Cl(6)	18(1)	26(1)	17(1)	10(1)	6(1)	9(1)
P(3)	14(1)	18(1)	18(1)	7(1)	8(1)	7(1)
P(4)	12(1)	14(1)	19(1)	5(1)	4(1)	5(1)
N(2)	16(2)	16(2)	22(2)	10(2)	9(2)	7(2)
C(24)	17(3)	25(3)	32(3)	12(3)	12(2)	12(3)
C(25)	28(3)	34(4)	35(4)	23(3)	13(3)	19(3)
C(26)	34(4)	26(3)	44(4)	18(3)	16(3)	17(3)
C(27)	21(3)	33(4)	42(4)	24(3)	12(3)	16(3)
C(28)	18(3)	17(3)	20(3)	7(2)	8(2)	3(2)
C(29)	25(3)	33(4)	23(3)	0(3)	10(3)	8(3)
C(30)	21(3)	25(3)	23(3)	8(3)	9(2)	3(3)
C(31)	23(3)	25(3)	25(3)	14(3)	9(3)	5(3)
C(32)	14(3)	25(3)	13(3)	5(2)	3(2)	4(2)
C(33)	17(3)	24(3)	16(3)	5(2)	5(2)	8(2)
C(34)	14(3)	21(3)	23(3)	2(2)	4(2)	0(2)
C(35)	30(3)	8(3)	33(3)	6(2)	8(3)	3(2)
C(36)	24(3)	24(3)	32(3)	9(3)	6(3)	10(3)
C(37)	20(3)	21(3)	16(3)	6(2)	6(2)	9(2)
C(38)	13(3)	12(3)	30(3)	11(2)	5(2)	3(2)
C(39)	17(3)	14(3)	16(3)	5(2)	5(2)	4(2)
C(40)	20(3)	23(3)	22(3)	0(2)	4(2)	5(3)
C(41)	17(3)	25(3)	32(3)	10(3)	5(3)	6(3)
C(42)	19(3)	21(3)	25(3)	7(2)	5(2)	1(2)
C(43)	15(3)	19(3)	17(3)	0(2)	2(2)	5(2)
C(44)	22(3)	24(3)	25(3)	8(3)	11(2)	8(3)
C(45)	21(3)	15(3)	29(3)	2(2)	9(2)	7(2)
C(46)	16(3)	27(3)	17(3)	-3(2)	4(2)	5(3)
C(47)	41(5)	33(4)	59(6)	-2(4)	19(4)	0(4)
Cl(7)	89(2)	60(2)	79(2)	-4(1)	49(2)	-10(2)
Cl(8)	33(1)	47(1)	58(1)	24(1)	7(1)	5(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C46 H86 Cl6 Ir2 N2 P4 * C1 H2 Cl2.

	x	y	z	U(eq)
H(2A)	8759	5506	5723	34
H(2B)	8875	4750	4905	34
H(2C)	9613	4990	5788	34
H(3A)	7445	3605	6586	35
H(3B)	7656	4765	6628	35
H(3C)	8703	4508	6816	35
H(4A)	8978	3191	5689	34
H(4B)	8319	2838	4753	34
H(4C)	7670	2385	5381	34
H(6A)	4917	1441	5487	38
H(6B)	6248	2164	5763	38
H(6C)	5642	1486	4808	38
H(7A)	4572	3036	6194	37
H(7B)	5102	4064	5957	37
H(7C)	5902	3759	6480	37
H(8A)	4287	1874	4071	47
H(8B)	4068	2877	4498	47
H(8C)	3637	1890	4795	47
H(9A)	5839	4906	5034	20
H(9B)	6958	5363	5747	20
H(11)	7830	7031	5507	27
H(12)	8895	7917	4733	26
H(13)	8913	6941	3414	27
H(15A)	8480	4631	2600	22
H(15B)	7962	5278	2225	22
H(17A)	6756	1698	1846	42
H(17B)	7974	2546	1878	42
H(17C)	7255	1560	1045	42
H(18A)	7508	2804	295	45
H(18B)	8177	3802	1129	45

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H(18C)	7095	3711	554	45
H(19A)	5156	2255	422	42
H(19B)	5026	1600	1026	42
H(19C)	5587	1357	268	42
H(21A)	6438	5758	2479	35
H(21B)	5611	5093	2927	35
H(21C)	5115	5424	2232	35
H(22A)	5286	4782	837	38
H(22B)	5613	3824	515	38
H(22C)	6559	4961	1106	38
H(23A)	3816	3696	1729	34
H(23B)	4230	2820	1769	34
H(23C)	4007	2999	916	34
H(25A)	10576	7598	2736	41
H(25B)	11685	8491	3421	41
H(25C)	11631	7362	2950	41
H(26A)	11818	6816	1668	47
H(26B)	12092	7535	1112	47
H(26C)	10833	6981	1204	47
H(27A)	13296	9442	3168	42
H(27B)	13505	9296	2261	42
H(27C)	13491	8450	2671	42
H(29A)	10051	8172	154	45
H(29B)	10958	7713	216	45
H(29C)	11044	8455	-312	45
H(30A)	12972	8942	956	38
H(30B)	13316	10159	1445	38
H(30C)	12996	9705	457	38
H(31A)	11506	10269	317	37
H(31B)	11966	10875	1294	37
H(31C)	10650	10133	905	37
H(32A)	12095	10410	3257	23
H(32B)	12722	10788	2590	23
H(34)	12650	12477	2916	28
H(35)	11569	13389	2750	31
H(36)	9608	12504	2471	32

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H(38A)	7981	10227	1554	22
H(38B)	7955	10940	2435	22
H(40A)	6653	7211	1158	37
H(40B)	6663	8037	727	37
H(40C)	5492	7190	772	37
H(41A)	4939	8567	1440	38
H(41B)	6077	9410	1351	38
H(41C)	5779	9565	2232	38
H(42A)	5016	7227	2041	36
H(42B)	5678	8220	2879	36
H(42C)	6208	7419	2538	36
H(44A)	8069	9564	4658	36
H(44B)	8169	8759	3862	36
H(44C)	6959	8688	3966	36
H(45A)	6199	9700	3433	34
H(45B)	7049	10851	3493	34
H(45C)	6965	10568	4311	34
H(46A)	9022	11470	3807	36
H(46B)	9621	10750	3939	36
H(46C)	9057	11197	4632	36
H(47A)	8032	6582	9572	65
H(47B)	8598	6068	10072	65

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C. X-Ray Diffraction Data for Ir(PNP)*$(I)_2$ (**3b**).

Table 1. Crystal data and structure refinement for C23 H42 I2 Ir N P2.

Identification code	periana24	
Empirical formula	C23 H42 I2 Ir N P2	
Formula weight	840.52	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.348(4) Å	α= 90°.
	b = 11.993(3) Å	β= 90.767(3)°.
	c = 16.442(4) Å	γ = 90°.
Volume	2828.9(12) $Å^3$	
Z	4	
Density (calculated)	1.974 Mg/m^3	
Absorption coefficient	7.026 mm^{-1}	
F(000)	1600	
Crystal size	0.15 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.42 to 28.33°.	
Index ranges	-19<=h<=19, -15<=k<=15, -21<=l<=21	
Reflections collected	27266	
Independent reflections	7019 [R(int) = 0.0363]	
Completeness to theta = 28.33°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.745 and 0.546	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7019 / 0 / 273	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0837	
R indices (all data)	R1 = 0.0441, wR2 = 0.0883	
Largest diff. peak and hole	2.797 and -0.811 $e.Å^{-3}$	

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C23 H42 I2 Ir N P2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	7475(1)	8805(1)	1479(1)	28(1)
I(1)	9058(1)	8715(1)	2572(1)	46(1)
I(2)	6356(1)	8143(1)	2676(1)	51(1)
P(1)	7560(1)	7041(1)	822(1)	32(1)
P(2)	7337(1)	10684(1)	1695(1)	35(1)
N(1)	8227(2)	9334(3)	485(2)	33(1)
C(1)	8571(4)	6097(4)	1047(3)	44(1)
C(2)	6474(4)	6158(4)	654(3)	43(1)
C(3)	7809(4)	7572(4)	-204(3)	42(1)
C(4)	8586(4)	5782(5)	1956(3)	55(1)
C(5)	8613(5)	5008(5)	546(4)	67(2)
C(6)	9468(3)	6764(5)	845(4)	56(2)
C(7)	5638(4)	6928(5)	548(4)	57(2)
C(8)	6294(4)	5424(5)	1386(4)	57(2)
C(9)	6530(4)	5433(5)	-112(4)	59(2)
C(10)	6323(3)	10740(5)	979(3)	45(1)
C(11)	7281(4)	11664(4)	2589(3)	49(1)
C(12)	8391(4)	11131(4)	1153(3)	45(1)
C(13)	6349(3)	9470(4)	782(3)	42(1)
C(14)	5380(4)	10985(6)	1366(4)	66(2)
C(15)	6450(4)	11469(6)	232(4)	62(2)
C(16)	6466(6)	11352(6)	3143(4)	75(2)
C(17)	7115(6)	12836(5)	2270(5)	89(2)
C(18)	8197(6)	11625(8)	3067(5)	98(3)
C(19)	8308(3)	8663(4)	-189(3)	38(1)
C(20)	8766(4)	9032(5)	-871(3)	52(1)
C(21)	9111(4)	10107(5)	-904(3)	54(1)
C(22)	8988(4)	10785(5)	-251(3)	49(1)
C(23)	8558(3)	10392(4)	443(3)	39(1)

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Table 3. Bond lengths [Å] and angles [°] for C23 H42 I2 Ir N P2.

Ir(1)-N(1)	2.072(4)
Ir(1)-C(13)	2.124(5)
Ir(1)-P(2)	2.2901(14)
Ir(1)-P(1)	2.3794(13)
Ir(1)-I(2)	2.6757(6)
Ir(1)-I(1)	2.8789(6)
P(1)-C(3)	1.841(5)
P(1)-C(1)	1.874(5)
P(1)-C(2)	1.901(5)
P(2)-C(12)	1.845(5)
P(2)-C(10)	1.861(5)
P(2)-C(11)	1.885(5)
N(1)-C(23)	1.357(6)
N(1)-C(19)	1.376(6)
C(1)-C(4)	1.542(7)
C(1)-C(5)	1.546(8)
C(1)-C(6)	1.555(7)
C(2)-C(8)	1.515(7)
C(2)-C(7)	1.522(8)
C(2)-C(9)	1.533(8)
C(3)-C(19)	1.492(7)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600

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C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-C(15)	1.521(8)
C(10)-C(14)	1.531(7)
C(10)-C(13)	1.557(7)
C(11)-C(17)	1.519(8)
C(11)-C(18)	1.522(9)
C(11)-C(16)	1.537(8)
C(12)-C(23)	1.488(7)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-C(20)	1.379(7)
C(20)-C(21)	1.382(8)
C(20)-H(20)	0.9300

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C(21)-C(22)	1.360(8)
C(21)-H(21)	0.9300
C(22)-C(23)	1.386(7)
C(22)-H(22)	0.9300

N(1)-Ir(1)-C(13)	81.89(17)
N(1)-Ir(1)-P(2)	82.39(11)
C(13)-Ir(1)-P(2)	69.38(14)
N(1)-Ir(1)-P(1)	83.28(11)
C(13)-Ir(1)-P(1)	97.57(14)
P(2)-Ir(1)-P(1)	161.83(4)
N(1)-Ir(1)-I(2)	174.52(10)
C(13)-Ir(1)-I(2)	92.82(14)
P(2)-Ir(1)-I(2)	97.13(3)
P(1)-Ir(1)-I(2)	96.07(3)
N(1)-Ir(1)-I(1)	95.09(10)
C(13)-Ir(1)-I(1)	159.88(14)
P(2)-Ir(1)-I(1)	90.52(3)
P(1)-Ir(1)-I(1)	101.83(3)
I(2)-Ir(1)-I(1)	90.37(2)
C(3)-P(1)-C(1)	103.4(2)
C(3)-P(1)-C(2)	103.2(2)
C(1)-P(1)-C(2)	108.8(2)
C(3)-P(1)-Ir(1)	96.95(17)
C(1)-P(1)-Ir(1)	119.47(17)
C(2)-P(1)-Ir(1)	120.93(17)
C(12)-P(2)-C(10)	108.8(3)
C(12)-P(2)-C(11)	103.9(2)
C(10)-P(2)-C(11)	115.4(2)
C(12)-P(2)-Ir(1)	97.95(17)
C(10)-P(2)-Ir(1)	90.31(18)
C(11)-P(2)-Ir(1)	137.67(18)
C(23)-N(1)-C(19)	118.2(4)
C(23)-N(1)-Ir(1)	120.9(3)
C(19)-N(1)-Ir(1)	120.5(3)
C(4)-C(1)-C(5)	108.1(5)

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C(4)-C(1)-C(6)	109.4(5)
C(5)-C(1)-C(6)	106.4(5)
C(4)-C(1)-P(1)	109.9(4)
C(5)-C(1)-P(1)	116.2(4)
C(6)-C(1)-P(1)	106.7(4)
C(8)-C(2)-C(7)	107.5(5)
C(8)-C(2)-C(9)	109.5(5)
C(7)-C(2)-C(9)	107.4(5)
C(8)-C(2)-P(1)	110.9(4)
C(7)-C(2)-P(1)	108.8(3)
C(9)-C(2)-P(1)	112.6(4)
C(19)-C(3)-P(1)	112.8(3)
C(19)-C(3)-H(3A)	109.0
P(1)-C(3)-H(3A)	109.0
C(19)-C(3)-H(3B)	109.0
P(1)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(1)-C(5)-H(5A)	109.5
C(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(1)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5

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C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(2)-C(8)-H(8A)	109.5
C(2)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(2)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(2)-C(9)-H(9A)	109.5
C(2)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(2)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(15)-C(10)-C(14)	110.0(5)
C(15)-C(10)-C(13)	113.0(5)
C(14)-C(10)-C(13)	107.4(5)
C(15)-C(10)-P(2)	115.5(4)
C(14)-C(10)-P(2)	115.6(4)
C(13)-C(10)-P(2)	94.4(3)
C(17)-C(11)-C(18)	109.7(6)
C(17)-C(11)-C(16)	108.3(5)
C(18)-C(11)-C(16)	110.2(6)
C(17)-C(11)-P(2)	108.4(4)
C(18)-C(11)-P(2)	109.7(4)
C(16)-C(11)-P(2)	110.5(4)
C(23)-C(12)-P(2)	110.4(3)
C(23)-C(12)-H(12A)	109.6
P(2)-C(12)-H(12A)	109.6
C(23)-C(12)-H(12B)	109.6
P(2)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(10)-C(13)-Ir(1)	105.9(3)

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C(10)-C(13)-H(13A)	110.5
Ir(1)-C(13)-H(13A)	110.5
C(10)-C(13)-H(13B)	110.5
Ir(1)-C(13)-H(13B)	110.5
H(13A)-C(13)-H(13B)	108.7
C(10)-C(14)-H(14A)	109.5
C(10)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(10)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(10)-C(15)-H(15A)	109.5
C(10)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(10)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(11)-C(17)-H(17A)	109.5
C(11)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(11)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(11)-C(18)-H(18A)	109.5
C(11)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(11)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(1)-C(19)-C(20)	120.9(5)

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N(1)-C(19)-C(3)	118.7(4)
C(20)-C(19)-C(3)	120.1(5)
C(19)-C(20)-C(21)	120.4(5)
C(19)-C(20)-H(20)	119.8
C(21)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	118.4(5)
C(22)-C(21)-H(21)	120.8
C(20)-C(21)-H(21)	120.8
C(21)-C(22)-C(23)	120.6(5)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
N(1)-C(23)-C(22)	121.3(5)
N(1)-C(23)-C(12)	117.2(4)
C(22)-C(23)-C(12)	121.4(5)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C23 H42 I2 Ir N P2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	27(1)	32(1)	25(1)	3(1)	0(1)	-2(1)
I(1)	44(1)	49(1)	45(1)	6(1)	-11(1)	-7(1)
I(2)	54(1)	58(1)	41(1)	2(1)	16(1)	-16(1)
P(1)	35(1)	34(1)	28(1)	1(1)	-2(1)	-2(1)
P(2)	39(1)	33(1)	34(1)	2(1)	1(1)	1(1)
N(1)	30(2)	39(2)	29(2)	6(2)	1(1)	-2(2)
C(1)	47(3)	40(3)	44(3)	3(2)	-1(2)	7(2)
C(2)	43(3)	40(3)	44(3)	0(2)	-8(2)	-11(2)
C(3)	52(3)	44(3)	29(2)	1(2)	-1(2)	-6(2)
C(4)	60(3)	52(3)	54(3)	11(3)	-12(3)	3(3)
C(5)	69(4)	49(4)	82(5)	-18(3)	-1(3)	15(3)
C(6)	35(3)	64(4)	67(4)	-8(3)	5(2)	8(3)
C(7)	45(3)	54(3)	73(4)	1(3)	-15(3)	-15(3)
C(8)	59(3)	54(3)	59(4)	6(3)	1(3)	-14(3)
C(9)	69(4)	56(4)	53(3)	-10(3)	-12(3)	-14(3)
C(10)	42(3)	47(3)	46(3)	2(2)	0(2)	6(2)
C(11)	66(4)	37(3)	45(3)	-7(2)	9(3)	0(3)
C(12)	47(3)	38(3)	50(3)	6(2)	6(2)	-6(2)
C(13)	36(2)	47(3)	41(3)	0(2)	-7(2)	3(2)
C(14)	41(3)	77(4)	80(5)	-7(4)	1(3)	15(3)
C(15)	61(4)	64(4)	62(4)	26(3)	-12(3)	7(3)
C(16)	111(6)	66(4)	48(4)	-6(3)	29(4)	-5(4)
C(17)	138(7)	43(4)	86(5)	-10(4)	18(5)	7(4)
C(18)	96(6)	114(6)	84(5)	-58(5)	-33(5)	29(5)
C(19)	35(2)	48(3)	31(2)	6(2)	1(2)	-1(2)
C(20)	59(3)	68(4)	29(3)	4(2)	12(2)	-2(3)
C(21)	56(3)	65(4)	41(3)	13(3)	15(2)	-7(3)
C(22)	47(3)	49(3)	51(3)	16(3)	9(2)	-5(2)
C(23)	35(2)	40(3)	41(3)	8(2)	2(2)	0(2)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C23 H42 I2 Ir N P2.

	x	y	z	U(eq)
H(3A)	8185	7029	-489	50
H(3B)	7227	7657	-504	50
H(4A)	8049	5337	2076	83
H(4B)	8577	6449	2280	83
H(4C)	9142	5366	2080	83
H(5A)	9190	4630	661	100
H(5B)	8576	5182	-23	100
H(5C)	8101	4535	688	100
H(6A)	10005	6368	1049	83
H(6B)	9441	7486	1095	83
H(6C)	9514	6848	266	83
H(7A)	5093	6493	422	86
H(7B)	5752	7441	112	86
H(7C)	5543	7336	1042	86
H(8A)	6294	5873	1869	86
H(8B)	6775	4870	1430	86
H(8C)	5700	5065	1321	86
H(9A)	5920	5161	-253	89
H(9B)	6939	4813	-9	89
H(9C)	6766	5869	-553	89
H(12A)	8314	11894	968	54
H(12B)	8925	11105	1520	54
H(13A)	6449	9352	206	50
H(13B)	5767	9117	930	50
H(14A)	5355	11755	1523	99
H(14B)	5306	10523	1838	99
H(14C)	4889	10830	981	99
H(15A)	5913	11401	-119	94
H(15B)	6995	11234	-53	94
H(15C)	6522	12232	397	94

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H(16A)	6530	10590	3312	113
H(16B)	5888	11443	2849	113
H(16C)	6471	11828	3612	113
H(17A)	6550	12851	1950	133
H(17B)	7629	13057	1938	133
H(17C)	7060	13343	2719	133
H(18A)	8172	12141	3513	147
H(18B)	8699	11825	2716	147
H(18C)	8296	10885	3273	147
H(20)	8844	8554	-1310	62
H(21)	9419	10361	-1362	65
H(22)	9195	11519	-270	59

1. (a) G.M. Sheldrick, *SHELXTL*, version 6.14; Bruker Analytical X-ray System, Inc.: Madison, WI, 1997 (b) R. H. Blessing, Acta Crystallogr. A51, 1995, **33**. (c) Internal Tables for Crystallographers, Vol. A, Space-Group Symmetry. D. Reidel Publishing Company, 1983, ISBN 90-277-1445-2.

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D. Computational Details

All energies discussed in this work are Gibbs free energies. For organometallic species these are calculated as:

$$G_{298K} = E_{elec} + G_{solv} + ZPVE + \sum_{\nu} \frac{h\nu}{e^{h\nu/kT} - 1} + \frac{n}{2}kT - T(S_{vib} + S_{rot} + S_{trans}),$$

where $n = 12$ accounts for the potential and kinetic energies of the translational and rotational modes and T = 298K. The values of $(S_{rot} + S_{trans})$ for each Ir intermediate were assumed to cancel. The free energies of gases were calculated with ideal gas statistical mechanics.

The geometry optimizations and zero-point vibrational energy (ZPVE) were carried out using the B3LYP functional[2] and the following basis: for Ir[3] and I[4], the Los Alamos angular momentum projected effective core potential (ECP) using the double-ζ contraction of valence functions; for Cl, 6-31G**++[5]; for P, 6-31G** with two *d*-functions ($\alpha_1 = .45$, $\alpha_2 = 1.35$) to allow core polarization; for others, 6-31G**. In order to obtain more accurate electronic energies, single-point energy calculations using the M06 functional[6] and a larger basis set were performed for E_{elec}, in which Ir was described with a triple-ζ contraction of the valence functions augmented with two *f* functions[7] and the core electrons were described by the same ECP, phosphorus was described by the 6-311+G-(3df) basis[8], iodine by the Los Alamos ECP with 3-ζ *s* and *p* functions, 3-ζ *d* functions ($\alpha_1 = 1.143$, $\alpha_2 = 0.35$, $\alpha_3 = 0.10$) and a single *f* function ($\alpha = 0.35$), and the other atoms were described with the 6-311++G** basis set.[9]

Solvation energies were calculated using the Poisson-Boltzmann self-consistent polarizable continuum method[10] implemented in Jaguar[11] to represent dimethylacetamide (dielectric constant = 38.85 and effective radius = 2.64 Å). The solvation calculations used the B3LYP/LACVP** level of theory and the gas-phase optimized structures.

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Cartesian Coordinates from DFT

3a [(PNP)IrI$_3$]

E(SCF) = -1778.28547693501

Ir1	-0.0088106397	0.0208091077	-0.0720193054
N2	-0.0479258004	-0.0085456469	2.0268472872
C3	1.0498181376	0.3820716124	2.7302127275
C4	1.0320498047	0.3825100714	4.1247870197
C5	-0.1043142181	-0.0437999348	4.8028731970
C6	-1.2119205798	-0.4533644249	4.0689509642
C7	-1.1726096141	-0.4180023570	2.6751947471
H8	1.9152751967	0.7078030594	4.6637270959
H9	-0.1263055645	-0.0572227008	5.8884690615
H10	-2.1157367981	-0.7928207027	4.5632904088
P11	2.4517491276	-0.1043283633	0.3530814232
P12	-2.4750761450	0.1190258205	0.2518724287
C13	-3.7621008590	-0.8345279799	-0.8653634194
C14	-3.3844420162	1.7424044782	0.8640578185
C15	3.3319048582	-1.7441802024	0.9730495188
C16	3.7865798088	0.8657618980	-0.6892974554
I17	-0.2017184595	-2.7704035135	-0.1354219102
I21	0.2019351657	2.8236666378	-0.0400411681
C22	2.2830136155	0.8135345844	1.9739652942
C23	-2.3720685451	-0.8340214790	1.8580720890
H17	3.1642593183	0.7228098519	2.6137785112
H18	2.1655673670	1.8688933903	1.7005089697
H19	-3.2800008858	-0.7589600889	2.4616724987
H20	-2.2406786352	-1.8830335414	1.5667299790
C24	3.4198288576	-2.8156494701	-0.1400760390
H25	4.1830382682	-2.5820012917	-0.8819411785
H26	3.6986249626	-3.7713328032	0.3209330596
H27	2.4725097570	-2.9655024818	-0.6542450957
C28	4.7640012627	-1.4999891722	1.5059246415
H29	5.4794847819	-1.2269609174	0.7306227237
H30	4.8047811352	-0.7487340108	2.3006987979
H31	5.1141951113	-2.4425349673	1.9446614947
C32	2.5465753896	-2.3114617128	2.1806905419
H33	2.9645351584	-3.2962975223	2.4217662136
H34	2.6677621879	-1.6891910555	3.0715443838
H35	1.4862200464	-2.4522869243	1.9804393679
C36	4.8424739712	1.5316007524	0.2228127949
H37	4.3924614348	2.2922689051	0.8676364489
H38	5.4021358062	0.8375079049	0.8472623033
H39	5.5657398431	2.0483335396	-0.4198269654
C40	4.4591427745	-0.1114894999	-1.6813547480
H41	5.0999664268	-0.8508357095	-1.2025862551

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H42	3.7207501745	-0.6296968023	-2.3005495712
H43	5.0944303286	0.4740388651	-2.3555208946
C44	3.1809555841	1.9916951553	-1.5512056718
H45	3.9768184262	2.3579483881	-2.2124268448
H46	2.3541604833	1.6490261706	-2.1742523532
H47	2.8341088191	2.8308346292	-0.9527725079
C48	-3.1236148038	-1.9455668398	-1.7232373347
H49	-2.8062705972	-2.7983313328	-1.1277081678
H50	-3.8922408855	-2.2947616219	-2.4247099419
H51	-2.2701294798	-1.5940336279	-2.3039082796
C52	-4.8541452330	-1.5169710955	-0.0094717330
H53	-4.4303629902	-2.2884152845	0.6403591351
H54	-5.4409688009	-0.8346554511	0.6028035889
H55	-5.5486850424	-2.0233550870	-0.6908138029
C56	-4.3935173899	0.1609101900	-1.8662812727
H57	-5.0032579908	-0.4117338403	-2.5742660630
H58	-5.0507506733	0.8943771372	-1.4011677158
H59	-3.6297820842	0.6864744981	-2.4473791087
C60	-3.4175187047	2.8359114047	-0.2301054989
H61	-4.1410167539	2.6165640498	-1.0148727102
H62	-3.7211318346	3.7818840012	0.2351604554
H63	-2.4451210617	2.9963531192	-0.6917315714
C64	-2.6560339827	2.2825673151	2.1190342925
H65	-1.5868925458	2.4232344709	1.9728426009
H66	-3.0817081572	3.2642072034	2.3594756947
H67	-2.8219616677	1.6428924459	2.9903160180
C68	-4.8399281939	1.4907006625	1.3252094911
H69	-5.2088810960	2.4252866371	1.7654886390
H70	-5.5195135683	1.2336587449	0.5130528604
H71	-4.9175550727	0.7244977524	2.1028542693
I72	0.0369813114	0.0617146792	-2.8121703918

3b [(PNP)*Ir(I)$_2$]

E(SCF) = -1766.29949789737

Ir1	0.0056784540	-0.1796075489	-0.0517207534
N2	0.1070849210	0.3352432137	1.9879660551
C3	1.1832505165	-0.0405258000	2.7304102657
C4	1.2546619205	0.2503382448	4.0925954409
C5	0.2197935984	0.9469850103	4.7047453847
C6	-0.8413181425	1.3876913000	3.9212733771
C7	-0.8661761971	1.0979577214	2.5577803721
H8	2.1194936882	-0.0802222058	4.6575265678
H9	0.2506398728	1.1638668353	5.7681824221
H10	-1.6453242039	1.9765787252	4.3495488740
P11	2.2856436567	-0.5103786068	0.2064993159
P12	-2.2342544585	0.7063669759	0.1294810747

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C13	-3.6985280922	-0.4277315218	0.6504484037
C14	-2.8849965134	2.0349184608	-1.1034888785
C15	3.6310639322	-1.7020675177	-0.4162105194
C16	2.5784755421	1.3181342598	-0.1791118465
I17	-0.4569935853	-2.9855357833	0.6242547283
C22	2.2954056771	-0.7846885992	2.0462303059
C23	-1.9151547470	1.7087446740	1.6660078360
H17	2.0797686614	-1.8573544804	2.1379940157
H18	3.2508760166	-0.5819919966	2.5391922704
H19	-1.5164895199	2.6682015039	1.3118161151
H20	-2.8194328100	1.9363353201	2.2367158773
C24	3.5857657306	-1.8067706417	-1.9546494208
H25	3.8207483983	-0.8640831219	-2.4507352357
H26	4.3341000464	-2.5428593021	-2.2727991643
H27	2.6060472846	-2.1381487356	-2.3057397340
C28	5.0158364143	-1.1968920349	0.0463777394
H29	5.2721850767	-0.2207268935	-0.3719691285
H30	5.0929797458	-1.1338291673	1.1370938377
H31	5.7794102162	-1.9092400959	-0.2894947543
C32	3.3982455882	-3.1145250598	0.1647238666
H33	4.1284427009	-3.7939933432	-0.2916660304
H34	3.5549448939	-3.1554693792	1.2469087068
H35	2.3954041533	-3.4891982263	-0.0508879379
C36	3.2866342483	2.1064538062	0.9344100812
H37	2.7928804081	1.9989291816	1.9048817612
H38	4.3335050035	1.8018081721	1.0491324107
H39	3.2795455905	3.1746677533	0.6828826009
C40	3.2897597465	1.5758366620	-1.5202243641
H41	4.3454359798	1.2879455977	-1.5093071627
H42	2.7883137254	1.0660857261	-2.3468567002
H43	3.2466367639	2.6525719564	-1.7264763323
C44	1.0549933157	1.6711114474	-0.3342858391
H45	0.8731826594	2.0855114348	-1.3239238907
H47	0.7566828424	2.4100784720	0.4192509298
C48	-3.3466912947	-1.0529449781	2.0197877513
H49	-3.3694527278	-0.3116560276	2.8262425397
H50	-4.1048622978	-1.8088519763	2.2577022866
H51	-2.3793164924	-1.5569481657	2.0173452292
C52	-5.0471496594	0.3000312223	0.8310400743
H53	-4.9929869900	1.1227659941	1.5520957433
H54	-5.4598568218	0.6814352310	-0.1045209600
H55	-5.7696413088	-0.4233976344	1.2287747361
C56	-3.8673127923	-1.5461602020	-0.4009604299
H57	-4.6415100009	-2.2421860447	-0.0543477293
H58	-4.1851365539	-1.1573397874	-1.3709933233
H59	-2.9457511624	-2.1135604214	-0.5403395111
C60	-3.6171255199	1.3542667634	-2.2810783959

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H61	-4.5670721435	0.9034930116	-1.9862808669
H62	-3.8410077424	2.1152037923	-3.0390828686
H63	-2.9939346517	0.5896201153	-2.7528519508
C64	-1.6839187342	2.8034825404	-1.6878712657
H65	-1.0270099080	2.1448390397	-2.2570272506
H66	-2.0668547932	3.5754974851	-2.3667372654
H67	-1.0956636750	3.3120720899	-0.9183325557
C68	-3.8135585964	3.0793667580	-0.4418091632
H69	-4.1174847271	3.8002943929	-1.2104791544
H70	-4.7227231823	2.6557530311	-0.0186356019
H71	-3.3046744547	3.6500392971	0.3416329716
I72	-0.1405778100	-0.6998862418	-2.7399521478

c [(PNP)*Ir(I)(H_2)$^+$]
E(SCF) = -1755.87216159333

Ir1	0.0258931824	-0.1574766425	0.0063347584
N2	0.0869250921	0.2988535391	2.0627325395
C3	1.1542052398	-0.0918908155	2.8103966182
C4	1.1952617014	0.1606974589	4.1804668612
C5	0.1395896866	0.8316020998	4.7876800903
C6	-0.9112649038	1.2878886556	3.9983442207
C7	-0.9081820267	1.0374275729	2.6277159107
H8	2.0506697184	-0.1743041311	4.7565426587
H9	0.1481656553	1.0198224720	5.8567117751
H10	-1.7252044346	1.8590338466	4.4307488278
P11	2.3220178290	-0.4860549684	0.3016753749
P12	-2.2568945809	0.6974589938	0.1775010258
C13	-3.7184925197	-0.4511872107	0.6609423044
C14	-2.8447502865	2.0118633567	-1.0926888861
C15	3.5952500894	-1.6960562166	-0.4076154982
C16	2.6159670007	1.3477242730	-0.0365636311
I17	-0.4756316188	-2.9375137106	0.4612157150
C22	2.2904024358	-0.8071505150	2.1273700381
C23	-1.9395716766	1.6710416808	1.7285955367
H17	2.1075332641	-1.8863801232	2.2032123674
H18	3.2367643658	-0.5912177221	2.6319101005
H19	-1.5357782353	2.6380136266	1.4010968527
H20	-2.8531975411	1.8884089434	2.2872517871
C24	3.3805939431	-1.8239060937	-1.9305077328
H25	3.5140253130	-0.8788140654	-2.4609761764
H26	4.1178286886	-2.5290670371	-2.3302185085
H27	2.3870478471	-2.2212832260	-2.1596279110
C28	5.0173905509	-1.1814679683	-0.0892525339
H29	5.2517129479	-0.2353776005	-0.5798999237
H30	5.1827399274	-1.0630755346	0.9867393034
H31	5.7420998336	-1.9224881544	-0.4446475608

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C32	3.4245431075	-3.0918853208	0.2319894651
H33	4.1099101163	-3.7792393328	-0.2763499541
H34	3.6945188342	-3.1000536561	1.2920437110
H35	2.4105152690	-3.4815382868	0.1231452797
C36	3.3896221186	2.0975344167	1.0590781817
H37	2.9463760756	1.9636753401	2.0505695144
H38	4.4373329736	1.7822003444	1.1062833923
H39	3.3785547458	3.1720274273	0.8407391506
C40	3.2572924162	1.6289298243	-1.4092541495
H41	4.3065306782	1.3312243593	-1.4653248390
H42	2.7141716681	1.1459183761	-2.2270786617
H43	3.2154958328	2.7094996557	-1.5876393709
C44	1.0979282380	1.7316843455	-0.1114768813
H45	0.8955963594	2.2814027193	-1.0269757964
H47	0.8072639877	2.3549278962	0.7380305050
C48	-3.3721838803	-1.1055994594	2.0189508548
H49	-3.3967578528	-0.3832897124	2.8411027174
H50	-4.1349199622	-1.8613226735	2.2369685393
H51	-2.4077645029	-1.6141615388	2.0145089601
C52	-5.0546590689	0.2988458289	0.8503613573
H53	-4.9884522173	1.1200527342	1.5712452887
H54	-5.4673324486	0.6831320024	-0.0839763396
H55	-5.7835654681	-0.4152158579	1.2507683822
C56	-3.9099313986	-1.5462793438	-0.4115390125
H57	-4.6887239710	-2.2366204910	-0.0674738901
H58	-4.2401915914	-1.1390859765	-1.3691248849
H59	-3.0024508813	-2.1297956928	-0.5707830768
C60	-3.5363026064	1.3096321851	-2.2816637821
H61	-4.5039779869	0.8815333013	-2.0161083769
H62	-3.7139797065	2.0483431711	-3.0711170646
H63	-2.9156337000	0.5166018285	-2.7124500898
C64	-1.6270533138	2.7744978164	-1.6491224052
H65	-0.9456359371	2.1180574519	-2.1942959083
H66	-1.9882754041	3.5345226789	-2.3509519824
H67	-1.0634619018	3.2967906863	-0.8715917017
C68	-3.7935152087	3.0629066248	-0.4715368327
H69	-4.0767667278	3.7745632049	-1.2552742389
H70	-4.7130206395	2.6405916172	-0.0715618863
H71	-3.3078741807	3.6419133894	0.3200383385
H73	0.0437786458	-0.0008633426	-1.6503413293
H74	-0.0996037101	-0.9141252991	-1.4737881524

d [(PNP)*Ir(I)$(H_2)^+$ hydrgenolysis TS]
E(SCF) = -1755.86116689784

Ir1	0.0239856669	-0.1455041930	-0.0399871281

N2	0.0824717158	0.3300675845	2.1259638591
C3	1.1645744262	-0.0296983158	2.8553089646
C4	1.2170682469	0.2301924833	4.2252368751
C5	0.1408016021	0.8661717159	4.8379182403
C6	-0.9391815571	1.2802606705	4.0621644862
C7	-0.9341446349	1.0251906105	2.6907362565
H8	2.0865335203	-0.0727273671	4.7986618415
H9	0.1540996561	1.0587961581	5.9063491276
H10	-1.7686952583	1.8195235259	4.5064680678
P11	2.3134096448	-0.4977746386	0.3070025231
P12	-2.2620764661	0.6722970543	0.1939391514
C13	-3.7173568638	-0.4984276819	0.6430436549
C14	-2.8577730363	2.0163332398	-1.0418524305
C15	3.6031461379	-1.7263336286	-0.3438616210
C16	2.6749108207	1.3139939268	-0.0831206489
I17	-0.4430685014	-2.8360355150	0.4252446677
C22	2.3022410815	-0.7365934411	2.1541356741
C23	-1.9813895637	1.6228735502	1.7785084243
H17	2.1540175625	-1.8160066344	2.2797310978
H18	3.2580790159	-0.4833988751	2.6232981816
H19	-1.6157259351	2.6128295819	1.4743709040
H20	-2.9120287947	1.7983246857	2.3241842528
C24	3.3876015984	-1.9231741419	-1.8594867484
H25	3.5343940263	-1.0063661513	-2.4335362464
H26	4.1160783442	-2.6561431865	-2.2233455468
H27	2.3869760569	-2.3108164052	-2.0704514563
C28	5.0243745919	-1.1969111089	-0.0463349155
H29	5.2599605485	-0.2715004157	-0.5748846577
H30	5.1908603097	-1.0358837547	1.0241028892
H31	5.7496688643	-1.9507826663	-0.3725005435
C32	3.4415835023	-3.0950254319	0.3561438312
H33	4.1348193495	-3.7970523887	-0.1202561735
H34	3.7083191588	-3.0566837475	1.4163667829
H35	2.4322654710	-3.4979995206	0.2587520063
C36	3.5465774969	2.0684678171	0.9342149644
H37	3.1688231379	1.9746644068	1.9568451371
H38	4.5816278203	1.7124831284	0.9161722992
H39	3.5632405076	3.1367308927	0.6872519074
C40	3.2300778970	1.5162430243	-1.5076230562
H41	4.2535155199	1.1550163264	-1.6199712336
H42	2.6069914787	1.0326506904	-2.2656410920
H43	3.2405109889	2.5906949242	-1.7250253096
C44	1.2005895222	1.8185423425	-0.0700194358
H45	1.0469877401	2.5839200839	-0.8340311730
H47	0.8888407284	2.2373176660	0.8848828513
C48	-3.3817914604	-1.1689917707	1.9966492570
H49	-3.4298989078	-0.4591903648	2.8286432152

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H50	-4.1371131637	-1.9385342221	2.1914001091
H51	-2.4101274943	-1.6623521100	2.0039370480
C52	-5.0652746449	0.2310808953	0.8314397808
H53	-5.0197047863	1.0364146010	1.5714101831
H54	-5.4711179854	0.6297906323	-0.0997401515
H55	-5.7890678060	-0.5016239861	1.2064410613
C56	-3.8893234151	-1.5737186593	-0.4524949716
H57	-4.6561433115	-2.2846257414	-0.1240532234
H58	-4.2265454832	-1.1490919458	-1.3999983899
H59	-2.9724483059	-2.1356746888	-0.6297457309
C60	-3.5168306316	1.3345880265	-2.2608059400
H61	-4.4813008623	0.8837654380	-2.0216166039
H62	-3.6956874894	2.0901798676	-3.0341414010
H63	-2.8732459510	0.5639365387	-2.6974629920
C64	-1.6481200310	2.8197389164	-1.5601116204
H65	-0.9715561161	2.2018241366	-2.1555166328
H66	-2.0182027682	3.6182344522	-2.2126590981
H67	-1.0836919405	3.3023241278	-0.7563572392
C68	-3.8321186384	3.0347138065	-0.4054496932
H69	-4.1260921236	3.7567179087	-1.1755841742
H70	-4.7445356803	2.5855171764	-0.0198430627
H71	-3.3638057887	3.6067401624	0.4016105828
H73	0.3007646266	0.9763543899	-1.1333291548
H74	-0.0656027009	-0.6891200100	-1.5261989793

e [(PNP)Ir(I)$_2$(H)]
E(SCF) = -1767.51831988294

Ir1	-0.0187389020	-0.1488820764	-0.0404626379
N2	-0.1565951865	0.0001609163	2.0448415122
C3	0.9376812019	0.3260617102	2.7837840993
C4	0.8959312004	0.2885153341	4.1759256764
C5	-0.2902880636	-0.0451884634	4.8219013805
C6	-1.4207825130	-0.3028319046	4.0551574754
C7	-1.3382651624	-0.2689524613	2.6635005833
H8	1.7893112392	0.5355733155	4.7392561809
H9	-0.3369478781	-0.0842710291	5.9059741641
H10	-2.3718167165	-0.5372799401	4.5210791445
P11	2.3299182243	0.0564402220	0.3521135749
P12	-2.3537502852	0.2200414024	0.1106022612
C13	-3.7339808073	-0.6197913695	-0.9314862015
C14	-2.7780999979	2.0885206517	0.3243357737
C15	3.4919718396	-1.4445087263	0.6401672067
C16	3.2730313611	1.4319467399	-0.6126833783
I17	-0.3039557484	-3.0426454904	0.3654882954
H21	0.0924262135	1.4033480528	-0.2245227290

C22	2.1572562349	0.8163251690	2.0498782360
C23	-2.5556111904	-0.5187777856	1.8104427205
H17	3.0520977558	0.7110534467	2.6685572272
H18	2.0165322317	1.8904414228	1.8724636736
H19	-3.4597603282	-0.2043389859	2.3405406296
H20	-2.6207100199	-1.5996382811	1.6259118315
C24	3.3939411680	-2.3787540168	-0.5855128199
H25	3.7756976877	-1.9084606289	-1.4953105791
H26	3.9988937646	-3.2745740534	-0.3964340050
H27	2.3659331809	-2.6980197526	-0.7662969917
C28	4.9722156452	-1.0887863854	0.8905613002
H29	5.4662250618	-0.6541234805	0.0199674422
H30	5.1070291134	-0.4158356095	1.7439747622
H31	5.5043291208	-2.0173616958	1.1312544451
C32	2.9965801217	-2.1889682822	1.9015168555
H33	3.5532020174	-3.1303087233	1.9850715767
H34	3.1924506102	-1.6184381423	2.8160786524
H35	1.9369003838	-2.4440132425	1.8520415384
C36	4.3991184019	2.0881289666	0.2204232859
H37	4.0171939265	2.5862989483	1.1172714350
H38	5.1808299370	1.3940691429	0.5236874184
H39	4.8731053054	2.8629570092	-0.3943022774
C40	3.8590940575	0.8490179819	-1.9175642485
H41	4.6657389458	0.1353342074	-1.7363386998
H42	3.0878144777	0.3631148395	-2.5211253886
H43	4.2801109577	1.6700917463	-2.5111509717
C44	2.2870328195	2.5552173315	-1.0027424290
H45	2.8554064905	3.3495412823	-1.5025576221
H46	1.5184665955	2.1995609595	-1.6900715868
H47	1.7961315124	3.0053859486	-0.1329177061
C48	-3.2604102084	-2.0158138581	-1.3840939485
H49	-3.0775608019	-2.6906910135	-0.5471046523
H50	-4.0528650684	-2.4525399373	-2.0053481280
H51	-2.3449586163	-1.9682668985	-1.9758244174
C52	-5.0355062381	-0.8128697466	-0.1197167385
H53	-4.8877265541	-1.4775507705	0.7369748798
H54	-5.4773084356	0.1175742699	0.2385755093
H55	-5.7741314653	-1.2952191689	-0.7712331102
C56	-4.0209629494	0.2035287918	-2.2064343382
H57	-4.7014890444	-0.3758621281	-2.8416906301
H58	-4.5093792615	1.1585522399	-2.0019590650
H59	-3.1084688128	0.3842968721	-2.7812185984
C60	-2.3637255842	2.8645201893	-0.9464745417
H61	-2.9598592346	2.5987222461	-1.8199126479
H62	-2.5030322008	3.9375351667	-0.7655474792
H63	-1.3138721866	2.6946597271	-1.1957563569
C64	-1.9630869486	2.6621182314	1.5065884072

H65	-0.8895076010	2.5224020774	1.3699904615
H66	-2.1565944164	3.7400344974	1.5661712704
H67	-2.2545308661	2.2286571036	2.4679161387
C68	-4.2644065804	2.3642808533	0.6348160189
H69	-4.3855756836	3.4355424732	0.8375321972
H70	-4.9273431913	2.1193489137	-0.1961470039
H71	-4.6118516404	1.8291438061	1.5248977482
I72	0.1133778625	-0.3125445322	-2.7734053471

$(P^{tBu}NP^{tBu})IrI_3$
E(SCF) = -1778.28547693501

Ir1	-0.0088106397	0.0208091077	-0.0720193054
N2	-0.0479258004	-0.0085456469	2.0268472872
C3	1.0498181376	0.3820716124	2.7302127275
C4	1.0320498047	0.3825100714	4.1247870197
C5	-0.1043142181	-0.0437999348	4.8028731970
C6	-1.2119205798	-0.4533644249	4.0689509642
C7	-1.1726096141	-0.4180023570	2.6751947471
H8	1.9152751967	0.7078030594	4.6637270959
H9	-0.1263055645	-0.0572227008	5.8884690615
H10	-2.1157367981	-0.7928207027	4.5632904088
P11	2.4517491276	-0.1043283633	0.3530814232
P12	-2.4750761450	0.1190258205	0.2518724287
C13	-3.7621008590	-0.8345279799	-0.8653634194
C14	-3.3844420162	1.7424044782	0.8640578185
C15	3.3319048582	-1.7441802024	0.9730495188
C16	3.7865798088	0.8657618980	-0.6892974554
I17	-0.2017184595	-2.7704035135	-0.1354219102
I21	0.2019351657	2.8236666378	-0.0400411681
C22	2.2830136155	0.8135345844	1.9739652942
C23	-2.3720685451	-0.8340214790	1.8580720890
H17	3.1642593183	0.7228098519	2.6137785112
H18	2.1655673670	1.8688933903	1.7005089697
H19	-3.2800008858	-0.7589600889	2.4616724987
H20	-2.2406786352	-1.8830335414	1.5667299790
C24	3.4198288576	-2.8156494701	-0.1400760390
H25	4.1830382682	-2.5820012917	-0.8819411785
H26	3.6986249626	-3.7713328032	0.3209330596
H27	2.4725097570	-2.9655024818	-0.6542450957
C28	4.7640012627	-1.4999891722	1.5059246415
H29	5.4794847819	-1.2269609174	0.7306227237
H30	4.8047811352	-0.7487340108	2.3006987979
H31	5.1141951113	-2.4425349673	1.9446614947
C32	2.5465753896	-2.3114617128	2.1806905419
H33	2.9645351584	-3.2962975223	2.4217662136
H34	2.6677621879	-1.6891910555	3.0715443838

H35	1.4862200464	-2.4522869243	1.9804393679
C36	4.8424739712	1.5316007524	0.2228127949
H37	4.3924614348	2.2922689051	0.8676364489
H38	5.4021358062	0.8375079049	0.8472623033
H39	5.5657398431	2.0483335396	-0.4198269654
C40	4.4591427745	-0.1114894999	-1.6813547480
H41	5.0999664268	-0.8508357095	-1.2025862551
H42	3.7207501745	-0.6296968023	-2.3005495712
H43	5.0944303286	0.4740388651	-2.3555208946
C44	3.1809555841	1.9916951553	-1.5512056718
H45	3.9768184262	2.3579483881	-2.2124268448
H46	2.3541604833	1.6490261706	-2.1742523532
H47	2.8341088191	2.8308346292	-0.9527725079
C48	-3.1236148038	-1.9455668398	-1.7232373347
H49	-2.8062705972	-2.7983313328	-1.1277081678
H50	-3.8922408855	-2.2947616219	-2.4247099419
H51	-2.2701294798	-1.5940336279	-2.3039082796
C52	-4.8541452330	-1.5169710955	-0.0094717330
H53	-4.4303629902	-2.2884152845	0.6403591351
H54	-5.4409688009	-0.8346554511	0.6028035889
H55	-5.5486850424	-2.0233550870	-0.6908138029
C56	-4.3935173899	0.1609101900	-1.8662812727
H57	-5.0032579908	-0.4117338403	-2.5742660630
H58	-5.0507506733	0.8943771372	-1.4011677158
H59	-3.6297820842	0.6864744981	-2.4473791087
C60	-3.4175187047	2.8359114047	-0.2301054989
H61	-4.1410167539	2.6165640498	-1.0148727102
H62	-3.7211318346	3.7818840012	0.2351604554
H63	-2.4451210617	2.9963531192	-0.6917315714
C64	-2.6560339827	2.2825673151	2.1190342925
H65	-1.5868925458	2.4232344709	1.9728426009
H66	-3.0817081572	3.2642072034	2.3594756947
H67	-2.8219616677	1.6428924459	2.9903160180
C68	-4.8399281939	1.4907006625	1.3252094911
H69	-5.2088810960	2.4252866371	1.7654886390
H70	-5.5195135683	1.2336587449	0.5130528604
H71	-4.9175550727	0.7244977524	2.1028542693
I72	0.0369813114	0.0617146792	-2.8121703918

($P^{tBu}NP^{tBu}$)IrI
E(SCF) = -1755.50928915354

Ir1	-0.0069798363	0.0093392322	0.0484628198
N2	-0.0480950815	-0.0110880624	2.1053148711
C3	1.0869472642	0.2192697037	2.8450837598
C4	1.0762132838	0.2024459499	4.2366719243
C5	-0.1063631198	-0.0327389827	4.9298938914

C6	-1.2593170813	-0.2576033846	4.1851738117
C7	-1.2125747968	-0.2534779158	2.7941820284
H8	2.0045310706	0.3911878078	4.7662328949
H9	-0.1287503803	-0.0407672815	6.0149258105
H10	-2.2085702251	-0.4545339805	4.6730830083
P11	2.2899437969	-0.0613830949	0.3453585899
P12	-2.3142638883	0.0720763071	0.2536265649
C13	-3.4607809269	-1.1403507892	-0.6844214498
C14	-3.0720642276	1.8270410993	0.3318431955
C15	3.0396615851	-1.8197462415	0.4191957136
C16	3.4756952742	1.1657537313	-0.5218996808
C22	2.3531859161	0.5460406134	2.1046393645
C23	-2.4465270825	-0.5701508891	1.9968126467
H17	3.2282068895	0.2096193809	2.6697493156
H18	2.4280680059	1.6377632141	2.0275580466
H19	-3.3453528275	-0.2482105849	2.5322894361
H20	-2.5130897693	-1.6604993858	1.8950430800
C24	2.8077564796	-2.5200828237	-0.9370454772
H25	3.3827580573	-2.0683948991	-1.7481694358
H26	3.1171535676	-3.5702082772	-0.8558244334
H27	1.7524841091	-2.4902704349	-1.2204519459
C28	4.5331810225	-1.8770038013	0.7897473000
H29	5.1726224035	-1.4540819807	0.0110479008
H30	4.7526421109	-1.3637006200	1.7324304892
H31	4.8308952682	-2.9257594816	0.9177134089
C32	2.2367231267	-2.5934878824	1.4901562483
H33	2.5538016964	-3.6437270590	1.4812424195
H34	2.4061654726	-2.2099736275	2.5016438102
H35	1.1638490258	-2.5561027524	1.2804202259
C36	4.7272635768	1.5107025400	0.3157184096
H37	4.4780659336	1.9880748907	1.2681956127
H38	5.3543372330	0.6423622586	0.5250443221
H39	5.3389159111	2.2262234066	-0.2480128775
C40	3.9237140390	0.6236699246	-1.8950176760
H41	4.6059958908	-0.2261155159	-1.8012623493
H42	3.0716386743	0.3277835528	-2.5121663828
H43	4.4653735863	1.4154537244	-2.4278564373
C44	2.6685210942	2.4645335745	-0.7498088565
H45	3.3209785962	3.2091671669	-1.2240227256
H46	1.8069903129	2.2908016683	-1.3973779819
H47	2.3032781089	2.8983112414	0.1876793594
C48	-2.6407425780	-2.4319666452	-0.9065836120
H49	-2.3105666761	-2.8833933672	0.0355889412
H50	-3.2715543208	-3.1687397242	-1.4206660597
H51	-1.7552874823	-2.2426897754	-1.5164601916
C52	-4.7428512920	-1.5054110864	0.0964757962
H53	-4.5292578454	-2.0035762464	1.0469784591

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H54	-5.3792248280	-0.6425936545	0.3007446257
H55	-5.3308625636	-2.2089773566	-0.5060898927
C56	-3.8564876185	-0.5718192818	-2.0629040819
H57	-4.3734061655	-1.3543599935	-2.6326705326
H58	-4.5454091054	0.2736522684	-1.9790673468
H59	-2.9818441312	-0.2606445862	-2.6397316375
C60	-2.7889543732	2.5546300223	-1.0000874556
H61	-3.3298496587	2.1175087248	-1.8420869272
H62	-3.1048365999	3.6021062221	-0.9104803342
H63	-1.7231643050	2.5331653464	-1.2419787955
C64	-2.3143850832	2.5813057231	1.4486970019
H65	-1.2338434816	2.5495235708	1.2814100145
H66	-2.6332344016	3.6310189692	1.4471852344
H67	-2.5232766192	2.1780621928	2.4450651130
C68	-4.5792453740	1.8731301885	0.6441169639
H69	-4.8853078320	2.9183722751	0.7807010968
H70	-5.1859204260	1.4638690734	-0.1674395465
H71	-4.8341152533	1.3407243272	1.5671613144
I72	0.0468694745	0.0408348740	-2.6820998484

$(P^{Me}NP^{Me})IrI_3$
E(SCF) = -1306.86049203421

Ir1	0.2618433890	-0.8140126590	0.0091621200
N2	0.3058583069	-0.1061046730	1.9976992852
C3	1.4276543808	0.4968953000	2.4772919826
C4	1.4794040919	0.9527545122	3.7936944172
C5	0.3648189452	0.8224659860	4.6147388142
C6	-0.7798057350	0.2200922967	4.1045643206
C7	-0.7872045837	-0.2560004853	2.7942723143
H8	2.3872574180	1.4233975474	4.1550223856
H9	0.3879144777	1.1852310984	5.6377134964
H10	-1.6658145015	0.0952946275	4.7175076135
C11	2.5925519341	0.7196482442	1.5401636270
H12	2.4742316297	1.7167194462	1.0959522383
H13	3.5386936587	0.7078124678	2.0908661860
C14	-1.9856058668	-1.0026658560	2.2544240763
H15	-1.8724036565	-2.0579877390	2.5352813988
H16	-2.9091231847	-0.6313128971	2.7103508449
P17	2.5707285824	-0.4576182684	0.1008968433
P18	-2.0364840091	-0.9978896980	0.3956311918
C19	-2.9708853233	-2.4967961309	-0.0739363653
H20	-2.4204935462	-3.3852913390	0.2390693942
H21	-3.9718190769	-2.4915417003	0.3686503613
H22	-3.0543470668	-2.5126096070	-1.1641260003
C23	-3.1965975253	0.3492228734	-0.0426266726

H24	-2.8329994321	1.3018298248	0.3454941088
H25	-3.2497414093	0.4322575150	-1.1312188765
H26	-4.1934591384	0.1333087360	0.3554764132
C27	3.7330618691	-1.7942753169	0.5639559790
H28	3.4000678014	-2.2832903502	1.4806311597
H29	3.7435628979	-2.5463422153	-0.2291810845
H30	4.7416278502	-1.3888414482	0.6952859687
C31	3.4631502854	0.3981352244	-1.2453500332
H32	3.5043547025	-0.2778219524	-2.1039151934
H33	2.9113601633	1.2917975905	-1.5408370603
H34	4.4803152424	0.6610183763	-0.9386535227
I35	0.5316924051	-3.4026100005	0.9957304943
I39	0.2049806512	-1.7285450802	-2.5584756123
I43	-0.0051106411	1.8202796981	-0.8483614912

$(P^{Me}NP^{Me})IrI$
E(SCF) = -1284.01479256409

Ir1	0.2391281198	-0.7728289195	-0.0218106988
N2	0.2883144530	-0.1261032538	1.9243453150
C3	1.4008526487	0.5021005462	2.4374595587
C4	1.4529524015	0.9314724217	3.7595819286
C5	0.3547017359	0.7661571512	4.5989438970
C6	-0.7773493700	0.1464409189	4.0768510721
C7	-0.7907342071	-0.3042446711	2.7608917360
H8	2.3569398143	1.4153534465	4.1155035913
H9	0.3801802114	1.1096917717	5.6280487956
H10	-1.6573061986	-0.0132944208	4.6918166696
C11	2.5543405227	0.7621199418	1.4992032106
H12	2.4385626630	1.7677254727	1.0717956851
H13	3.5078649826	0.7492080356	2.0389028797
C14	-1.9811892137	-1.0572172493	2.2184468282
H15	-1.8686087574	-2.1204452740	2.4717388895
H16	-2.9094015751	-0.7107809087	2.6864740333
P17	2.4825469104	-0.3969944176	0.0485050250
P18	-1.9931382529	-0.9958881448	0.3612596179
C19	-2.9706573849	-2.4689792929	-0.1309267052
H20	-2.4534059823	-3.3716852304	0.2035269302
H21	-3.9861524962	-2.4490981177	0.2787155425
H22	-3.0172513236	-2.4980535845	-1.2229414021
C23	-3.1217747812	0.3976019935	-0.0536877489
H24	-2.7047207341	1.3264438259	0.3439476291
H25	-3.1759702125	0.4914964274	-1.1419143339
H26	-4.1303040756	0.2468348041	0.3468988200
C27	3.6155812422	-1.7770048620	0.4952938509
H28	3.2341588459	-2.2784473735	1.3885198640
H29	3.6211674319	-2.5033089075	-0.3222746976

H30	4.6385964165	-1.4298626734	0.6776193029
C31	3.4109724629	0.4772148093	-1.2712804315
H32	3.4082323146	-0.1529653703	-2.1647983375
H33	2.8931802101	1.4070948622	-1.5192921844
H34	4.4439354428	0.6935345306	-0.9786779883
I39	0.1736692808	-1.6206946103	-2.5845578818

$(P^{tBu}NP^{tBu})IrCl_3$
E(SCF) = -3124.81516577335

Ir1	-0.0061613223	0.0153540106	-0.0257575616
N2	-0.0498395732	-0.0059440910	2.0405665041
C3	1.0535901819	0.3749039603	2.7399059765
C4	1.0373571498	0.3711380694	4.1343665488
C5	-0.1088672312	-0.0339937932	4.8108747520
C6	-1.2250677695	-0.4249212440	4.0781811541
C7	-1.1819243588	-0.4004121010	2.6844797318
H8	1.9250443937	0.6815070665	4.6748702861
H9	-0.1319806454	-0.0449709176	5.8964869093
H10	-2.1348080009	-0.7458492572	4.5740228416
P11	2.4051594529	-0.0892151060	0.3303996619
P12	-2.4295057618	0.1135338894	0.2297282989
C13	-3.6137151515	-0.8883179013	-0.9217280002
C14	-3.3026474937	1.7733859958	0.7088254729
C15	3.2584003473	-1.7585152922	0.8128991231
C16	3.6369354804	0.9366867403	-0.7481345727
Cl17	-0.1879576952	-2.4141727072	0.0177462794
Cl21	0.1730101601	2.4433788697	0.0751430122
C22	2.2824938359	0.8015555843	1.9702581509
C23	-2.3767215808	-0.8109081114	1.8546987339
H17	3.1738555973	0.7010850250	2.5952985857
H18	2.1659420783	1.8581045878	1.7023393309
H19	-3.2940456736	-0.7232025373	2.4430292243
H20	-2.2479239026	-1.8617271854	1.5703469174
C24	3.1780047205	-2.7740106881	-0.3503156086
H25	3.7791388600	-2.4758669659	-1.2096187360
H26	3.5710196575	-3.7352381724	0.0044880196
H27	2.1513995125	-2.9293796882	-0.6799423976
C28	4.7378378325	-1.5890925224	1.2247001365
H29	5.3883844666	-1.3122466771	0.3943011042
H30	4.8742354901	-0.8626106188	2.0325720628
H31	5.0936324861	-2.5557500051	1.6020760732
C32	2.5352637019	-2.3516896654	2.0456066565
H33	2.9600516957	-3.3443293818	2.2385997766
H34	2.7024830948	-1.7539843351	2.9467834968
H35	1.4658640486	-2.4775535728	1.8831034876
C36	4.7962622011	1.5202571800	0.0907904231

H37	4.4325374969	2.2107634942	0.8581062866
H38	5.4213205587	0.7695202205	0.5722540590
H39	5.4410435854	2.1018419399	-0.5792096328
C40	4.1832745856	0.0365379794	-1.8799711523
H41	4.8482336298	-0.7524712813	-1.5256595209
H42	3.3715306954	-0.4138983919	-2.4590685140
H43	4.7648137423	0.6649654128	-2.5646456709
C44	2.9338033254	2.1253019139	-1.4364466204
H45	3.6647499426	2.5854953282	-2.1137122733
H46	2.0676925225	1.8135091136	-2.0205692793
H47	2.6086258258	2.8848553154	-0.7270117640
C48	-2.8809469910	-2.0614581570	-1.6056039222
H49	-2.5863843744	-2.8371088094	-0.9001823175
H50	-3.5816957891	-2.5057178071	-2.3241674374
H51	-1.9902227700	-1.7368755814	-2.1441906914
C52	-4.8064904106	-1.4895693169	-0.1442434447
H53	-4.4744530836	-2.1979663236	0.6211491401
H54	-5.4505302923	-0.7493132034	0.3284716235
H55	-5.4236305676	-2.0548934507	-0.8530760557
C56	-4.1137111529	0.0359312407	-2.0555003172
H57	-4.6642061335	-0.5780163084	-2.7778917555
H58	-4.7948669977	0.8160346519	-1.7127423304
H59	-3.2792051649	0.5003003901	-2.5893263770
C60	-3.1724761068	2.8114868348	-0.4296798239
H61	-3.7361807735	2.5308734603	-1.3197455344
H62	-3.5803433058	3.7658973601	-0.0732101227
H63	-2.1326444539	2.9725226235	-0.7117836278
C64	-2.6328426092	2.3417787581	1.9826627666
H65	-1.5574150154	2.4696375520	1.8686215777
H66	-3.0653075736	3.3309688068	2.1763669600
H67	-2.8387507448	1.7270411442	2.8641561014
C68	-4.7982927594	1.5969699949	1.0539458959
H69	-5.1706601117	2.5572682176	1.4316394190
H70	-5.4126732805	1.3337170626	0.1921328879
H71	-4.9685675655	0.8574865453	1.8433819676
Cl72	0.0448493089	0.0409865276	-2.4388189717

($P^{tBu}NP^{tBu}$)*$IrCl_2$
E(SCF) = -2663.96912174219

Ir1	0.0249422008	-0.1481078990	-0.0437214091
N2	0.0990362750	0.3330753517	1.9777378760
C3	1.1646347762	-0.0585205623	2.7305436516
C4	1.2279987205	0.2303514436	4.0932385233
C5	0.1960141985	0.9381859264	4.6983258355
C6	-0.8587708668	1.3831880870	3.9088320686
C7	-0.8797307037	1.0934688977	2.5453640272

H8	2.0854895874	-0.1085355054	4.6646211147
H9	0.2229085586	1.1567927930	5.7614975315
H10	-1.6643048545	1.9722421631	4.3340237107
P11	2.2762786819	-0.5165345222	0.2159868661
P12	-2.2277198529	0.6645484629	0.1214597473
C13	-3.6226734633	-0.5467149489	0.6353048006
C14	-2.9006855279	1.9322341763	-1.1456935998
C15	3.4869030324	-1.7928767168	-0.4758655610
C16	2.6079298503	1.3093755203	-0.1600778683
Cl17	-0.4564696493	-2.6145193458	0.5407981165
C22	2.2762184798	-0.8143127714	2.0518115472
C23	-1.9441552323	1.6838501926	1.6537554021
H17	2.0479135195	-1.8841106452	2.1315657565
H18	3.2296117293	-0.6283925097	2.5556341561
H19	-1.5712670771	2.6519525847	1.2948349911
H20	-2.8526544812	1.8879591709	2.2272379949
C24	3.3889150927	-1.8161851253	-2.0167029202
H25	3.7656759721	-0.8993267519	-2.4732008273
H26	4.0014993111	-2.6455359700	-2.3905181857
H27	2.3594596190	-1.9658724499	-2.3512537422
C28	4.9263360040	-1.4619632961	-0.0285585615
H29	5.2709765218	-0.4958170210	-0.4076456251
H30	5.0310933673	-1.4595263287	1.0620353578
H31	5.6062630757	-2.2301563650	-0.4171871841
C32	3.0897498305	-3.1908916541	0.0525660130
H33	3.7012395528	-3.9391522922	-0.4661052593
H34	3.2865033794	-3.3034314919	1.1235210006
H35	2.0351859436	-3.4129817435	-0.1291316259
C36	3.3153739355	2.0727217400	0.9706637467
H37	2.8063426638	1.9670335728	1.9335186147
H38	4.3542619182	1.7447069651	1.0965982641
H39	3.3343591860	3.1431011322	0.7291739623
C40	3.3516104115	1.5555659894	-1.4838543264
H41	4.3965019526	1.2294169293	-1.4524806715
H42	2.8503438611	1.0690480241	-2.3238532439
H43	3.3501904302	2.6347839631	-1.6820808514
C44	1.0877386142	1.6838742274	-0.3315418015
H45	0.9200704657	2.0817863075	-1.3318935326
H47	0.7981716068	2.4442233775	0.4052257010
C48	-3.2308310104	-1.1593604892	2.0005278984
H49	-3.2675364187	-0.4219561655	2.8101766093
H50	-3.9613702446	-1.9397923823	2.2466549511
H51	-2.2469301452	-1.6301475166	1.9722415929
C52	-5.0078905715	0.1085604761	0.8089390281
H53	-4.9976684077	0.9419107386	1.5202581757
H54	-5.4362577981	0.4593652647	-0.1322698698
H55	-5.6940241415	-0.6465659702	1.2122920192

C56	-3.7166045118	-1.6794207373	-0.4116719039
H57	-4.4506950888	-2.4167590592	-0.0626152458
H58	-4.0528288022	-1.3189370457	-1.3863024305
H59	-2.7590013837	-2.1880112499	-0.5353611276
C60	-3.5515933141	1.1837307729	-2.3296562991
H61	-4.4928380084	0.7005892615	-2.0576284708
H62	-3.7757759941	1.9085652479	-3.1221348790
H63	-2.8744447812	0.4323489524	-2.7458675061
C64	-1.7063811998	2.7298719325	-1.7065449762
H65	-1.0087075991	2.0765187135	-2.2316474390
H66	-2.0891543188	3.4730047466	-2.4173270782
H67	-1.1614163765	3.2742192795	-0.9289560936
C68	-3.8996764329	2.9423255418	-0.5396045785
H69	-4.2069791115	3.6407314123	-1.3277061838
H70	-4.8035029773	2.4787770165	-0.1459084150
H71	-3.4484452628	3.5424202844	0.2575588789
Cl72	-0.0732713366	-0.5714231374	-2.4273036466

$(P^{tBu}NP^{tBu})IrCl$
E(SCF) = -2204.34344554301

Ir1	-0.1514226561	-0.3375123051	0.0656896449
N2	-0.0094492043	0.2648824341	2.0049631359
C3	1.2129307124	0.4024926319	2.6246156357
C4	1.3236996454	0.8110368955	3.9499884034
C5	0.1877845164	1.1154564997	4.6937165878
C6	-1.0487552749	0.9848614957	4.0691219218
C7	-1.1319198738	0.5551928438	2.7486549710
H8	2.3141066729	0.9005911270	4.3853221376
H9	0.2635861601	1.4427977111	5.7257216748
H10	-1.9680275652	1.2010762851	4.6045054723
C11	2.4520370697	0.1409803918	1.8076051362
H12	2.8002944049	1.0967446260	1.3965114862
H13	3.2582392769	-0.2406666187	2.4427793953
C14	-2.4776294975	0.3464214281	2.1041185538
H15	-2.8257447801	-0.6626790301	2.3580126945
H16	-3.2140293510	1.0454270050	2.5140383762
P17	2.0667163663	-0.9175289609	0.3244561701
P18	-2.3426535636	0.3634088056	0.2471301839
C19	-3.7627218237	-0.7891737461	-0.2923719693
C20	-2.6706781040	2.1766865619	-0.2542721937
C21	2.3757447421	-2.7112836272	0.9027474867
C22	3.3670551103	-0.3506230722	-0.9507459473
Cl23	-0.3187086259	-1.0426521727	-2.2438131971
C25	1.5655012303	-2.8952575394	2.2066479451
H26	1.9586375456	-2.2969151736	3.0349912277

H27	0.5144370343	-2.6321727626	2.0567511630
H28	1.6168318935	-3.9481401273	2.5104744937
C29	3.8479710079	-3.0635376581	1.1827598899
H30	4.3143999446	-2.3779000278	1.8990331727
H31	3.9017697783	-4.0700776706	1.6174752999
H32	4.4531842489	-3.0730783888	0.2727170525
C33	4.7780371061	-0.1444266197	-0.3600934909
H34	4.7926550086	0.6069387211	0.4360086916
H35	5.2136588926	-1.0642856256	0.0343511247
H36	5.4435823566	0.2180948587	-1.1535989550
C37	1.7907218486	-3.6764752847	-0.1519134314
H38	1.8314054833	-4.7020435347	0.2375701700
H39	0.7491835008	-3.4296673496	-0.3747837116
H40	2.3453700926	-3.6582716546	-1.0924345615
C41	3.4354924621	-1.3533035501	-2.1217159293
H42	3.9021716363	-2.2990625158	-1.8309417850
H43	2.4424823449	-1.5570096711	-2.5317090317
H44	4.0501202071	-0.9223770988	-2.9221173818
C45	2.8618920300	1.0012382456	-1.5071193908
H46	3.5802148190	1.3683023738	-2.2517359700
H47	1.8850911017	0.8939569415	-1.9830526845
H48	2.7769400016	1.7678997403	-0.7290205246
C49	-3.2618160413	-2.2325100575	-0.0526183539
H50	-3.0350844893	-2.4267353584	1.0015468217
H51	-4.0500202983	-2.9350945161	-0.3532076548
H52	-2.3623540814	-2.4416280523	-0.6351442078
C53	-5.0726520472	-0.5841889361	0.4980850385
H54	-4.9445307130	-0.7547273999	1.5718700404
H55	-5.5016345887	0.4102948683	0.3619913420
H56	-5.8152179703	-1.3111750696	0.1457750348
C57	-2.2831285681	2.3561476921	-1.7386412561
H58	-2.9564025121	1.8267060150	-2.4160105834
H59	-2.3261568772	3.4227947262	-1.9946979603
H60	-1.2689289197	1.9935376454	-1.9265408737
C61	-4.1102207509	2.6698338957	-0.0201868763
H62	-4.8300031716	2.1803071924	-0.6811342892
H63	-4.4400719478	2.5254849721	1.0147410821
H64	-4.1610096052	3.7465668861	-0.2277170464
C65	-1.7066895017	3.0421732095	0.5897104465
H66	-1.7733479437	4.0827512740	0.2487419341
H67	-1.9551727401	3.0315191466	1.6559518191
H68	-0.6719022306	2.7078666284	0.4713075057
C69	-4.0372013298	-0.6237131814	-1.8019342663
H70	-4.7246704084	-1.4151332675	-2.1261688781
H71	-4.5148626187	0.3327863445	-2.0338534898
H72	-3.1182591443	-0.7144790768	-2.3875334922

Electronic Supplementary Information for Dalton Transactions
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$(P^{Me}NP^{Me})IrCl_3$
E(SCF) = -2653.35508626093

Ir1	0.2613498036	-0.8150597846	0.0056132581
N2	0.3053103083	-0.1184266209	1.9669027371
C3	1.4165783049	0.5120306677	2.4369510829
C4	1.4682961256	0.9692827009	3.7528927093
C5	0.3638173600	0.8112008019	4.5834497857
C6	-0.7704273598	0.1802400331	4.0833037749
C7	-0.7774314907	-0.2956431755	2.7730051443
H8	2.3674399434	1.4615957977	4.1070849039
H9	0.3866744681	1.1745734155	5.6062673474
H10	-1.6477642548	0.0342630709	4.7040229838
C11	2.5667213265	0.7512275745	1.4851153820
H12	2.4058722287	1.7252260455	1.0053160987
H13	3.5168147943	0.7943398732	2.0271686011
C14	-1.9610385215	-1.0651844923	2.2317240815
H15	-1.8057779668	-2.1258380062	2.4673923754
H16	-2.8881317277	-0.7433674436	2.7167266781
P17	2.5599192630	-0.4687423528	0.0836345209
P18	-2.0268569453	-1.0016558626	0.3758717228
C19	-2.9201287788	-2.5049550286	-0.1392107184
H20	-2.3247092968	-3.3750068917	0.1451577606
H21	-3.9187490578	-2.5591617799	0.3053189839
H22	-3.0030537750	-2.4918136645	-1.2293268084
C23	-3.1327127055	0.3874908509	-0.0509501492
H24	-2.7068425965	1.3195127990	0.3256549676
H25	-3.1856910441	0.4676053147	-1.1399633877
H26	-4.1372930589	0.2340075489	0.3559527426
C27	3.6684041028	-1.8309848358	0.5841970693
H28	3.2713044064	-2.3116483686	1.4803791872
H29	3.6800947421	-2.5799856402	-0.2120682764
H30	4.6857361268	-1.4686454741	0.7632794327
C31	3.4111584773	0.3617381200	-1.2981211086
H32	3.4522523064	-0.3365937993	-2.1383752777
H33	2.8149430840	1.2243575473	-1.6028295358
H34	4.4252952077	0.6707650967	-1.0263925509
Cl35	0.4846544146	-3.0838778723	0.8736886188
Cl39	0.2100612684	-1.6206618857	-2.2615033663
Cl43	0.0407854699	1.4957986201	-0.7434584852

$(P^{Me}NP^{Me})IrCl$
E(SCF) = -1732.84412030560

Ir1	0.2615292093	-0.8142336464	0.0085304995

N2	0.3042705406	-0.1330515215	1.9266010336
C3	1.4184449229	0.4992413654	2.4358044896
C4	1.4667019704	0.9526844017	3.7495246503
C5	0.3638225823	0.8117352277	4.5872639918
C6	-0.7694093961	0.1898392037	4.0704771402
C7	-0.7798009737	-0.2870085498	2.7642104740
H8	2.3724683161	1.4374281719	4.0999180262
H9	0.3867079014	1.1747513874	5.6096071511
H10	-1.6536715517	0.0474008988	4.6836384806
C11	2.5790782188	0.7364461360	1.4989919731
H12	2.4708970618	1.7340681073	1.0511865822
H13	3.5292711499	0.7291641389	2.0445772183
C14	-1.9733628723	-1.0451294126	2.2335312767
H15	-1.8691994896	-2.1032619897	2.5108978163
H16	-2.9011619629	-0.6819623609	2.6894925261
P17	2.5081860272	-0.4503742088	0.0725317374
P18	-1.9754100388	-1.0239205937	0.3766547727
C19	-2.9245100161	-2.5181304001	-0.1063373256
H20	-2.4036294859	-3.4070895693	0.2578553320
H21	-3.9507283927	-2.5053551547	0.2760512627
H22	-2.9422992619	-2.5680434663	-1.1986134835
C23	-3.1140975922	0.3475354428	-0.0819206005
H24	-2.7109747000	1.2904007055	0.2966500670
H25	-3.1591251092	0.4144986156	-1.1726172688
H26	-4.1249115986	0.1959202365	0.3126354433
C27	3.6485579753	-1.8189746859	0.5355380739
H28	3.2750348263	-2.3070294125	1.4394777097
H29	3.6515387547	-2.5589216318	-0.2698092272
H30	4.6717155805	-1.4658176304	0.7052870447
C31	3.4155980577	0.3926288322	-1.2813343114
H32	3.3909397282	-0.2576791869	-2.1601813284
H33	2.8957047663	1.3185870045	-1.5392770273
H34	4.4557556070	0.6110575218	-1.0170564003
Cl39	0.2108010627	-1.6161977200	-2.2522880935

$(P^{tBu}NP^{tBu})Ir(OH)_3$
E(SCF) = -1971.54236640380

Ir1	3.3966306464	0.8192243925	-0.0495072874
N2	1.3189994664	0.8622938477	-0.0295047202
C3	0.6469683322	1.9702262311	0.3813284086
C4	-0.7456854634	2.0150870828	0.3500418714
C5	-1.4585173613	0.9129219143	-0.1147490534
C6	-0.7586129398	-0.2147906322	-0.5342030986
C7	0.6347423166	-0.2229710751	-0.4817361858
H8	-1.2561733280	2.9107466818	0.6879450064
H9	-2.5437659907	0.9326906621	-0.1490533905

H10	-1.2800101896	-1.0917516619	-0.9031162427
C11	1.4802916578	3.1190596781	0.8849970125
H12	0.9056449470	4.0496921081	0.8916574096
H13	1.7790865303	2.8839832606	1.9117576833
C14	1.4455217535	-1.4110492975	-0.9300135532
H15	0.8370680699	-2.3190870104	-0.9426245961
H16	1.8039972315	-1.1906772069	-1.9445380291
P17	3.1022262759	3.1986219769	-0.0378671206
P18	3.0427719122	-1.5250065628	0.0286800467
C19	2.5879900991	-2.2895655159	1.7231432260
C20	4.1205968481	-2.7425585007	-0.9865132720
C21	4.2816987835	4.2695979105	1.0460959446
C22	2.6838204637	4.0704643324	-1.6884947814
O23	3.2595928895	0.6547297694	-2.1399141263
H24	4.1797625711	0.5948869379	-2.4252755780
O26	3.5658164110	0.9722134383	2.0322333639
H27	4.5279854588	0.8816168435	2.1135440451
C28	1.6438625817	3.2017763596	-2.4367343681
H29	2.0030363692	2.1754206249	-2.5542777547
H30	0.6701926518	3.2083230283	-1.9369516472
H31	1.4942982175	3.6407364784	-3.4321043567
C32	2.0850630833	5.4875874567	-1.5538446543
H33	1.2440861038	5.5199977092	-0.8525950911
H34	2.8081621266	6.2436943216	-1.2528581807
H35	1.6915479037	5.7861656577	-2.5333021288
C36	3.9698840388	4.1055162933	-2.5405346293
H37	3.7469242564	4.5562318168	-3.5157313420
H38	4.7686917785	4.6975020599	-2.0824931083
H39	4.3317527576	3.0886657641	-2.7168962336
C40	4.2224647809	5.7905618075	0.8085658480
H41	4.5720730717	6.0792284627	-0.1857668352
H42	3.2208916908	6.2023108732	0.9623470579
H43	4.8874192650	6.2742830508	1.5356010832
C44	3.9657377682	4.0130321542	2.5377745958
H45	3.0374177757	4.5097685997	2.8425095680
H46	3.8860542171	2.9433840243	2.7495172508
H47	4.7744962443	4.4447397799	3.1410506328
C48	5.7178124307	3.7791052180	0.7516748931
H49	6.4213315530	4.3287565088	1.3896588519
H50	5.8293835426	2.7101572657	0.9490199236
H51	6.0088405750	3.9683053182	-0.2880392515
C52	4.8026421914	-1.9586191865	-2.1283135600
H53	4.0783553942	-1.5165457410	-2.8140679330
H54	5.4246904859	-1.1585325767	-1.7174747779
H55	5.4366439202	-2.6565123673	-2.6907026029
C56	3.2887693376	-3.8870736967	-1.6037740763
H57	2.5464638149	-3.5128536854	-2.3151338871

H58	3.9624768223	-4.5495685445	-2.1618274159
H59	2.7732626421	-4.4973508060	-0.8594381441
C60	5.2494593847	-3.3274970980	-0.1111552693
H61	5.9280911519	-3.8974352843	-0.7579106043
H62	5.8361084940	-2.5367350916	0.3650724694
H63	4.8865006397	-4.0125823938	0.6581311343
C64	2.0988596325	-3.7483468874	1.6297272651
H65	1.2498592821	-3.8624888136	0.9465332684
H66	2.8839246851	-4.4422496634	1.3206192427
H67	1.7581079819	-4.0684457873	2.6226781747
C68	1.4577869545	-1.4372097230	2.3454466202
H69	0.5229738370	-1.4966430630	1.7806212888
H70	1.2521744632	-1.8288579760	3.3499483084
H71	1.7755300702	-0.3972197280	2.4431187168
C72	3.7963284478	-2.1851843883	2.6815106010
H73	3.4941206553	-2.5660158418	3.6658812631
H74	4.6609547744	-2.7654975981	2.3582613820
H75	4.0797318169	-1.1368610820	2.7914346126
O76	5.4424887142	0.6144693598	-0.0689368464
H77	5.8178755653	1.3521488212	-0.5633343370

($P^{tBu}NP^{tBu}$)Ir(OH)
E(SCF) = -1819.90691657755

Ir1	-0.1569733927	-0.3338715980	0.0603603627
N2	-0.0001240816	0.2513771990	2.0106442395
C3	1.2261274124	0.3948132087	2.6274470598
C4	1.3463830082	0.7951731079	3.9522483210
C5	0.2140125749	1.0907755823	4.7087047134
C6	-1.0272876429	0.9576554998	4.0891359237
C7	-1.1197936060	0.5348469312	2.7688628546
H8	2.3401344955	0.8888363694	4.3800159611
H9	0.2954942368	1.4129054631	5.7416708173
H10	-1.9436902903	1.1675955756	4.6327288998
C11	2.4521430346	0.1517983937	1.7832719173
H12	2.7667572731	1.1094702399	1.3485662632
H13	3.2837751210	-0.2081155070	2.3981021634
C14	-2.4702813751	0.3195925155	2.1272730708
H15	-2.8089140126	-0.6974738275	2.3642574214
H16	-3.2123789455	1.0060119301	2.5482628113
P17	2.0448257994	-0.9275218331	0.3204073955
P18	-2.3392073669	0.3669127266	0.2719081294
C19	-3.7155900708	-0.8038843097	-0.3257469045
C20	-2.6811645039	2.1806983093	-0.2152366023
C21	2.3651205884	-2.7145586332	0.9218873130
C22	3.3406826689	-0.3988121680	-0.9857512974
O23	-0.4788364293	-0.8417204167	-1.8774199053

H24	0.3252181004	-1.1694342868	-2.2937759329
C25	1.5634107511	-2.8792137702	2.2335060815
H26	1.9647631128	-2.2718502690	3.0509657538
H27	0.5136149134	-2.6089356087	2.0868080230
H28	1.6099736708	-3.9290483440	2.5496448993
C29	3.8389561599	-3.0637217981	1.1961688956
H30	4.3076061725	-2.3684670996	1.9011407760
H31	3.8978532358	-4.0644819850	1.6433006754
H32	4.4415916839	-3.0836028787	0.2843283591
C33	4.7512318537	-0.1449912636	-0.4148981389
H34	4.7544637604	0.6451374778	0.3420494313
H35	5.1961251528	-1.0387124747	0.0273730296
H36	5.4140117708	0.1849269581	-1.2252420428
C37	1.7684115027	-3.6957383239	-0.1104881911
H38	1.7966328285	-4.7143769670	0.2969781579
H39	0.7270252522	-3.4416515657	-0.3286356109
H40	2.3221954603	-3.7062217334	-1.0523536393
C41	3.4312119781	-1.4479459955	-2.1133706430
H42	3.9044227752	-2.3770423310	-1.7854256274
H43	2.4485463195	-1.6948088224	-2.5277104679
H44	4.0376216493	-1.0446386854	-2.9339943450
C45	2.8064602177	0.9143290578	-1.6040792907
H46	3.5128092984	1.2659719670	-2.3678963787
H47	1.8265891879	0.7658113921	-2.0651012988
H48	2.6991433380	1.7107471107	-0.8603280497
C49	-3.1909029845	-2.2394892429	-0.0907800162
H50	-2.9845222158	-2.4451022954	0.9650930276
H51	-3.9556575230	-2.9544334992	-0.4226133308
H52	-2.2721947106	-2.4088684431	-0.6563947096
C53	-5.0596782825	-0.6330934712	0.4094543846
H54	-4.9674228412	-0.8070004364	1.4867971657
H55	-5.5020005591	0.3542314816	0.2632192615
H56	-5.7743254236	-1.3720763921	0.0250600981
C57	-2.2674017566	2.3808309024	-1.6906604756
H58	-2.9499954203	1.8890732930	-2.3871736132
H59	-2.2724079608	3.4535380971	-1.9240246071
H60	-1.2639223283	1.9861529783	-1.8729322005
C61	-4.1289359019	2.6570730455	-0.0005647925
H62	-4.8310670840	2.1670048466	-0.6799691328
H63	-4.4750006716	2.4949849684	1.0265669268
H64	-4.1890842604	3.7356951083	-0.1959467451
C65	-1.7376860041	3.0424245738	0.6549519803
H66	-1.8062238188	4.0868696755	0.3264391404
H67	-2.0005149223	3.0148103041	1.7170509289
H68	-0.6991277410	2.7164035562	0.5478834867
C69	-3.9053104606	-0.6239854672	-1.8465267888
H70	-4.5478387390	-1.4298668332	-2.2239800742

H71	-4.3958152484	0.3217940886	-2.0946440375
H72	-2.9433980567	-0.6807941138	-2.3652421235

$(P^{Me}NP^{Me})Ir(OH)_3$
E(SCF) = -1500.06044810485

Ir1	-0.0126330858	0.0315089326	0.0225877422
N2	-0.0023344098	-0.0579128201	2.1050925929
C3	1.1716411932	0.0186587285	2.7908999238
C4	1.1961289629	-0.0477966664	4.1819340956
C5	0.0013516362	-0.1614984986	4.8879831396
C6	-1.1953368989	-0.2215094752	4.1780061628
C7	-1.1761679812	-0.1836551770	2.7857060468
H8	2.1482872005	0.0083491412	4.6989968790
H9	0.0025907835	-0.2023575388	5.9729486417
H10	-2.1460551766	-0.3157778798	4.6921494359
C11	2.4162637023	0.2215361343	1.9686156116
H12	2.4846579431	1.2922044609	1.7304932881
H13	3.3161728558	-0.0884579332	2.5090159323
C14	-2.4281681614	-0.3253060733	1.9584312329
H15	-2.4992664292	-1.3762043613	1.6460359405
H16	-3.3226148781	-0.0544596872	2.5280465558
P17	2.2120199879	-0.5334347348	0.2867067925
P18	-2.2292117982	0.5479431696	0.3351147396
C19	-3.5215927762	-0.1662841933	-0.7370837262
H20	-3.2746937994	-1.2227625111	-0.8656375607
H21	-4.5279543298	-0.0565529272	-0.3213188247
H22	-3.4726387469	0.3220480254	-1.7139589660
C23	-2.6622045199	2.3083819663	0.5897028958
H24	-2.7995275865	2.7773777171	-0.3893390101
H25	-3.5698057393	2.4501246193	1.1841687743
H26	-1.8019772904	2.7868054475	1.0664377753
C27	2.6087864065	-2.3159340164	0.4186618291
H28	1.7144894685	-2.8105634547	0.8084102902
H29	2.7885562539	-2.7117280912	-0.5856963691
H30	3.4814112592	-2.5231048025	1.0452198374
C31	3.5628549243	0.2389758102	-0.6800886440
H32	3.5932838741	-0.1969669310	-1.6831311467
H33	3.3197816337	1.3017555033	-0.7623428753
H34	4.5438117669	0.1136316958	-0.2108239846
O35	0.6950379721	2.0095485839	0.1196561408
H37	0.5281656982	2.3226163242	-0.7811067791
O39	-0.7060728307	-1.9462585483	-0.0615140599
H40	-0.7444146978	-2.0666435590	-1.0227678328
O41	-0.1843639084	0.1268468101	-2.0081190737
H42	0.6985946254	0.2197326086	-2.3847872637

Electronic Supplementary Information for Dalton Transactions
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($P^{Me}NP^{Me}$)Ir(OH)
E(SCF) = -1348.40794648830

Ir1	0.0082607154	0.0469717365	0.0216603284
N2	-0.0151885771	-0.0078268787	2.0731270374
C3	1.1544356322	-0.0910022861	2.8041533684
C4	1.1573013848	-0.1064230389	4.1927879493
C5	-0.0389615366	-0.0735436996	4.9076225173
C6	-1.2235692179	-0.0072018018	4.1760644041
C7	-1.1952825557	0.0410576736	2.7887734848
H8	2.1106906487	-0.1667231080	4.7090664011
H9	-0.0475363076	-0.0983913005	5.9921799786
H10	-2.1856492244	0.0292789019	4.6782528309
C11	2.4442288033	-0.2291115116	2.0298884566
H12	3.2828404749	0.2109672907	2.5807878400
H13	2.6649253934	-1.2981345951	1.8993739805
C14	-2.4637016283	0.2079041689	1.9907570734
H15	-3.3179207600	-0.2499557517	2.5018043524
H16	-2.6787436435	1.2805959531	1.8851364330
P17	2.2352183241	0.4305138412	0.3110226050
P18	-2.2079550317	-0.3969687124	0.2565437416
C19	-2.7741425168	-2.1521152152	0.2903939903
H20	-2.1254092231	-2.7162523698	0.9649707208
H21	-3.8155915595	-2.2492616698	0.6173579885
H22	-2.6708362011	-2.5825086031	-0.7098861713
C23	-3.5735163814	0.4166136051	-0.6793952968
H24	-3.5557264399	0.0685380996	-1.7169515125
H25	-4.5585267014	0.1934282883	-0.2551567601
H26	-3.4140423347	1.4978830584	-0.6827167085
C27	3.5194264796	-0.4230050860	-0.6857491011
H28	3.3329493643	-1.4996017315	-0.6647844754
H29	3.4173495076	-0.0878980948	-1.7217835504
H30	4.5357581257	-0.2153184575	-0.3339652709
C31	2.8678173923	2.1587724562	0.3771814400
H32	2.7713225347	2.6048588510	-0.6168385971
H33	2.2490658425	2.7377461953	1.0675020830
H34	3.9155779319	2.2078808725	0.6942073679
O35	0.2061610776	0.1337973811	-1.9727685150
H36	-0.6580280762	0.1399383181	-2.3993156482