Supplementary Material

Reactions of the Binuclear Complexes, $[MIr(CO)_3(Ph_2PCH_2PPh_2)_2]$ (M = Rh, Ir) with Alkyl Halides: Dramatic Reactivity Differences as a Function of Metal Combination and Alkyl Halide.

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Table S–1. Crystallographic Experimental Details for Compound **4**.

A. Crystal Data	
formula	$C_{54.7}H_{50.25}Cl_2I_{1.15}Ir_2O_{2.85}P_4$
formula weight	1478.31
crystal dimensions (mm)	0.34 × 0.12 × 0.06
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	20.0497 (9)
b (Å)	13.9589 (6)
c (Å)	20.9456 (8)
β (deg)	112.732 (3)
V (Å^3)	5406.7 (4)
Z	4
ρ_{calcd} (g cm^{-3})	1.816
μ (mm^{-1})	16.89
B. Data Collection and Refinement Conditions	
diffractometer	Siemens P4/RA[b]
radiation (λ [Å])	graphite-monochromated Cu Kα (1.54178)
temperature (°C)	–60
scan type	θ–2θ
data collection 2θ limit (deg)	113.5
total data collected	7450 ($0 \le h \le 21$, $0 \le k \le 15$, $-22 \le l \le 20$)
independent reflections	7213
number of observations (*NO*)	5827 ($F_o^2 \ge 2\sigma(F_o^2)$)
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.4129–0.1633
data/restraints/parameters	7213 / 0 / 613
goodness-of-fit (S)[e]	1.060 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
$F_o^2 > 2\sigma(F_o^2)$	$\boldsymbol{R_1}$ **= 0.0552,** wR_2 = 0.1330
all data	R_1 = 0.0725, $\boldsymbol{wR_2}$ **= 0.1444**
largest difference peak and hole	2.282 and –1.976 e Å^{-3}

(continued)

Table S–1. Crystallographic Experimental Details for Compound **4** (continued)

[a]Obtained from least-squares refinement of 28 reflections with $56.9° < 2\theta < 57.9°$.

[b]Programs for diffractometer operation and data collection were those of the XSCANS system supplied by Siemens.

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted R-factors wR_2 and all goodnesses of fit S are based on F_o^2; conventional R-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. R-factors based on F_o^2 are statistically about twice as large as those based on F_o, and R-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0832P)^2 + 25.9490P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S–2. Atomic Coordinates and Displacement Parameters for Compound **4**.

(a) 'inner-sphere' atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ir(1)	0.22518(3)	0.13984(3)	-0.01806(2)	0.0297(2)*
Ir(2)	0.23828(3)	-0.03795(3)	-0.07937(2)	0.0307(2)*
I(1)	0.37430(5)	0.15697(7)	0.01617(5)	0.0530(3)*
I(2)[a]	0.2433(5)	-0.2009(5)	-0.1476(5)	0.049(2)*
P(1)	0.2030(2)	0.2193(2)	-0.12180(15)	0.0304(6)*
P(2)	0.2329(2)	0.0328(2)	-0.18036(15)	0.0305(6)*
P(3)	0.2579(2)	0.0712(2)	0.09112(14)	0.0313(7)*
P(4)	0.2681(2)	-0.1181(2)	0.02287(15)	0.0313(7)*
O(1)	0.1389(6)	0.2886(7)	0.0184(5)	0.065(3)*
O(2)	0.0963(5)	0.0119(6)	-0.0858(4)	0.048(2)*
O(3)[b]	0.2196(6)	-0.1793(8)	-0.1903(7)	0.040(3)*
C(1)	0.1752(7)	0.2352(10)	0.0068(6)	0.047(3)*
C(2)	0.1587(6)	0.0284(9)	-0.0695(6)	0.037(3)*
C(3)[b]	0.2586(11)	-0.1655(13)	-0.1197(11)	0.046(5)*
C(4)[b]	0.2396(13)	-0.2610(11)	-0.2150(9)	0.076(7)*
C(5)	0.2497(6)	0.1637(7)	-0.1702(6)	0.034(3)*
C(6)	0.3063(6)	-0.0416(8)	0.0994(6)	0.034(3)*

(b) dppm phenyl carbons

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(11)	0.2338(8)	0.3425(8)	-0.1127(6)	0.043(3)*
C(12)	0.1929(11)	0.4124(10)	-0.0985(9)	0.072(5)*
C(13)	0.2179(14)	0.5091(11)	-0.0875(10)	0.090(7)*
C(14)	0.2803(13)	0.5305(11)	-0.0940(9)	0.082(6)*
C(15)	0.3206(11)	0.4636(12)	-0.1097(9)	0.076(5)*
C(16)	0.2983(8)	0.3697(10)	-0.1180(8)	0.059(4)*
C(21)	0.1089(7)	0.2316(8)	-0.1809(6)	0.037(3)*
C(22)	0.0916(8)	0.2672(9)	-0.2464(7)	0.049(3)*
C(23)	0.0198(8)	0.2773(10)	-0.2925(8)	0.058(4)*
C(24)	-0.0339(7)	0.2522(10)	-0.2706(8)	0.057(4)*
C(25)	-0.0193(8)	0.2203(10)	-0.2063(8)	0.057(4)*
C(26)	0.0523(6)	0.2076(9)	-0.1601(7)	0.045(3)*
C(31)	0.1514(6)	0.0257(8)	-0.2583(6)	0.033(3)*
C(32)	0.0915(6)	-0.0200(9)	-0.2546(6)	0.037(3)*
C(33)	0.0274(8)	-0.0227(10)	-0.3132(7)	0.053(4)*
C(34)	0.0219(8)	0.0191(10)	-0.3735(7)	0.055(4)*
C(35)	0.0809(8)	0.0646(10)	-0.3778(7)	0.054(4)*
C(36)	0.1448(7)	0.0681(9)	-0.3209(6)	0.041(3)*
C(41)	0.3072(7)	-0.0049(8)	-0.2044(7)	0.038(3)*

Table S–2. Atomic Coordinates and Displacement Parameters for Compound **4** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(42)	0.2997(8)	-0.0497(9)	-0.2651(7)	0.048(3)*
C(43)	0.3582(9)	-0.0775(11)	-0.2781(9)	0.067(5)*
C(44)	0.4286(10)	-0.0630(12)	-0.2293(10)	0.077(5)*
C(45)	0.4376(8)	-0.0203(12)	-0.1663(9)	0.072(5)*
C(46)	0.3762(7)	0.0094(11)	-0.1535(8)	0.055(4)*
C(51)	0.1848(6)	0.0446(8)	0.1195(6)	0.037(3)*
C(52)	0.1122(7)	0.0524(9)	0.0752(7)	0.044(3)*
C(53)	0.0576(7)	0.0330(11)	0.0963(8)	0.055(4)*
C(54)	0.0731(7)	0.0024(9)	0.1634(7)	0.049(3)*
C(55)	0.1442(7)	-0.0075(10)	0.2091(6)	0.046(3)*
C(56)	0.1999(7)	0.0147(9)	0.1874(7)	0.046(3)*
C(61)	0.3213(6)	0.1418(9)	0.1631(5)	0.033(3)*
C(62)	0.3724(7)	0.1000(9)	0.2202(6)	0.043(3)*
C(63)	0.4169(8)	0.1542(11)	0.2771(7)	0.058(4)*
C(64)	0.4102(8)	0.2510(11)	0.2759(8)	0.059(4)*
C(65)	0.3576(8)	0.2966(10)	0.2166(8)	0.059(4)*
C(66)	0.3128(7)	0.2400(9)	0.1628(7)	0.048(3)*
C(71)	0.1969(6)	-0.1900(8)	0.0339(6)	0.035(3)*
C(72)	0.2044(7)	-0.2314(10)	0.0966(7)	0.049(3)*
C(73)	0.1492(10)	-0.2857(13)	0.1010(9)	0.074(5)*
C(74)	0.0874(10)	-0.2983(14)	0.0474(11)	0.097(7)*
C(75)	0.0791(10)	-0.2607(15)	-0.0155(10)	0.103(8)*
C(76)	0.1340(8)	-0.2045(10)	-0.0216(7)	0.061(4)*
C(81)	0.3429(7)	-0.2002(8)	0.0384(6)	0.037(3)*
C(82)	0.3403(8)	-0.2967(10)	0.0486(7)	0.052(4)*
C(83)	0.3976(10)	-0.3580(12)	0.0544(8)	0.072(5)*
C(84)	0.4578(10)	-0.3181(14)	0.0481(8)	0.070(5)*
C(85)	0.4620(8)	-0.2213(16)	0.0392(9)	0.080(6)*
C(86)	0.4060(7)	-0.1621(11)	0.0332(7)	0.056(4)*
(c) solvent dichloromethane atoms				
Atom	*x*	*y*	*z*	U_{eq}, Å^2
Cl(1)	0.4294(3)	0.6740(4)	-0.2504(4)	0.135(3)*
Cl(2)	0.4984(6)	0.5927(5)	-0.1119(5)	0.178(4)*
C(91)	0.4782(13)	0.6937(16)	-0.1596(12)	0.131(10)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.15. [b]Refined with an occupancy factor of 0.85.

Table S–3. Selected Interatomic Distances for Compound **4** (Å)

(a) involving 'inner-sphere' atoms

Atom1	Atom2	Distance
Ir(1)	Ir(2)	2.8527(7)
Ir(1)	I(1)	2.8025(10)
Ir(1)	P(1)	2.324(3)
Ir(1)	P(3)	2.328(3)
Ir(1)	C(1)	1.858(15)
Ir(1)	C(2)	2.061(13)
Ir(2)	I(2)	2.708(8)
Ir(2)	P(2)	2.299(3)
Ir(2)	P(4)	2.281(3)
Ir(2)	C(2)	1.924(12)
Ir(2)	C(3)	2.08(2)
P(1)	C(5)	1.801(12)
P(2)	C(5)	1.855(11)
P(3)	C(6)	1.822(11)
P(4)	C(6)	1.829(11)
O(1)	C(1)	1.13(2)
O(2)	C(2)	1.185(14)
O(3)	C(3)	1.39(2)
O(3)	C(4)	1.37(2)

(b) involving dppm phenyl carbons

Atom1	Atom2	Distance
P(1)	C(11)	1.812(12)
P(1)	C(21)	1.822(12)
P(2)	C(31)	1.812(11)
P(2)	C(41)	1.826(12)
P(3)	C(51)	1.821(11)
P(3)	C(61)	1.838(11)
P(4)	C(71)	1.832(12)
P(4)	C(81)	1.814(12)
C(11)	C(12)	1.38(2)
C(11)	C(16)	1.39(2)
C(12)	C(13)	1.43(2)
C(13)	C(14)	1.35(3)
C(14)	C(15)	1.35(3)
C(15)	C(16)	1.37(2)
C(21)	C(22)	1.37(2)
C(21)	C(26)	1.40(2)
C(22)	C(23)	1.40(2)
C(23)	C(24)	1.37(2)
C(24)	C(25)	1.34(2)
C(25)	C(26)	1.40(2)
C(31)	C(32)	1.39(2)
C(31)	C(36)	1.40(2)
C(32)	C(33)	1.39(2)
C(33)	C(34)	1.36(2)
C(34)	C(35)	1.38(2)
C(35)	C(36)	1.37(2)
C(41)	C(42)	1.37(2)
C(41)	C(46)	1.40(2)
C(42)	C(43)	1.36(2)
C(43)	C(44)	1.40(2)
C(44)	C(45)	1.40(2)
C(45)	C(46)	1.42(2)
C(51)	C(52)	1.40(2)
C(51)	C(56)	1.40(2)
C(52)	C(53)	1.36(2)
C(53)	C(54)	1.39(2)
C(54)	C(55)	1.38(2)
C(55)	C(56)	1.39(2)
C(61)	C(62)	1.37(2)
C(61)	C(66)	1.38(2)
C(62)	C(63)	1.40(2)
C(63)	C(64)	1.36(2)
C(64)	C(65)	1.43(2)
C(65)	C(66)	1.38(2)
C(71)	C(72)	1.39(2)
C(71)	C(76)	1.36(2)
C(72)	C(73)	1.37(2)
C(73)	C(74)	1.32(2)
C(74)	C(75)	1.37(2)
C(75)	C(76)	1.40(2)
C(81)	C(82)	1.37(2)
C(81)	C(86)	1.41(2)
C(82)	C(83)	1.40(2)
C(83)	C(84)	1.38(2)
C(84)	C(85)	1.37(3)
C(85)	C(86)	1.36(2)

(c) within the solvent dichloromethane molecule

Atom1	Atom2	Distance
Cl(1)	C(91)	1.79(2)
Cl(2)	C(91)	1.68(2)

Table S–4. Selected Interatomic Angles for Compound **4** (deg)

(a) involving 'inner-sphere' atoms

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ir(2)	Ir(1)	I(1)	85.10(3)	I(2)	Ir(2)	P(4)	92.0(2)
Ir(2)	Ir(1)	P(1)	90.67(7)	I(2)	Ir(2)	C(2)	131.5(4)
Ir(2)	Ir(1)	P(3)	92.51(7)	P(2)	Ir(2)	P(4)	167.54(11)
Ir(2)	Ir(1)	C(1)	154.6(4)	P(2)	Ir(2)	C(2)	98.4(3)
Ir(2)	Ir(1)	C(2)	42.4(3)	P(2)	Ir(2)	C(3)	86.6(6)
I(1)	Ir(1)	P(1)	89.88(8)	P(4)	Ir(2)	C(2)	93.6(3)
I(1)	Ir(1)	P(3)	85.17(8)	P(4)	Ir(2)	C(3)	86.6(6)
I(1)	Ir(1)	C(1)	120.3(4)	C(2)	Ir(2)	C(3)	139.2(7)
I(1)	Ir(1)	C(2)	127.5(3)	Ir(1)	P(1)	C(5)	111.6(4)
P(1)	Ir(1)	P(3)	173.86(10)	Ir(2)	P(2)	C(5)	112.1(4)
P(1)	Ir(1)	C(1)	89.5(4)	Ir(1)	P(3)	C(6)	112.8(4)
P(1)	Ir(1)	C(2)	91.2(3)	Ir(2)	P(4)	C(6)	113.9(4)
P(3)	Ir(1)	C(1)	89.9(4)	C(3)	O(3)	C(4)	112.8(15)
P(3)	Ir(1)	C(2)	94.7(3)	Ir(1)	C(1)	O(1)	173.5(13)
C(1)	Ir(1)	C(2)	112.2(5)	Ir(1)	C(2)	Ir(2)	91.4(5)
Ir(1)	Ir(2)	I(2)	175.3(2)	Ir(1)	C(2)	O(2)	134.0(10)
Ir(1)	Ir(2)	P(2)	93.46(7)	Ir(2)	C(2)	O(2)	134.6(10)
Ir(1)	Ir(2)	P(4)	92.31(7)	Ir(2)	C(3)	O(3)	115.6(12)
Ir(1)	Ir(2)	C(2)	46.2(4)	P(1)	C(5)	P(2)	112.1(6)
Ir(1)	Ir(2)	C(3)	174.4(6)	P(3)	C(6)	P(4)	113.2(6)
I(2)	Ir(2)	P(2)	82.7(2)				

(b) involving dppm phenyl carbons

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ir(1)	P(1)	C(11)	114.8(4)	P(1)	C(21)	C(22)	120.6(10)
Ir(1)	P(1)	C(21)	117.0(4)	P(1)	C(21)	C(26)	121.1(9)
C(5)	P(1)	C(11)	103.8(6)	C(22)	C(21)	C(26)	118.3(12)
C(5)	P(1)	C(21)	106.6(6)	C(21)	C(22)	C(23)	121.6(14)
C(11)	P(1)	C(21)	101.7(6)	C(22)	C(23)	C(24)	118.4(14)
Ir(2)	P(2)	C(31)	120.7(4)	C(23)	C(24)	C(25)	121.8(14)
Ir(2)	P(2)	C(41)	112.1(4)	C(24)	C(25)	C(26)	120.4(14)
C(5)	P(2)	C(31)	102.6(5)	C(21)	C(26)	C(25)	119.5(13)
C(5)	P(2)	C(41)	100.6(5)	P(2)	C(31)	C(32)	118.2(8)
C(31)	P(2)	C(41)	106.5(6)	P(2)	C(31)	C(36)	123.2(9)
Ir(1)	P(3)	C(51)	116.6(4)	C(32)	C(31)	C(36)	118.5(11)
Ir(1)	P(3)	C(61)	115.3(4)	C(31)	C(32)	C(33)	119.2(11)
C(6)	P(3)	C(51)	105.0(5)	C(32)	C(33)	C(34)	121.6(13)
C(6)	P(3)	C(61)	102.2(5)	C(33)	C(34)	C(35)	119.8(13)
C(51)	P(3)	C(61)	103.3(5)	C(34)	C(35)	C(36)	119.8(12)
Ir(2)	P(4)	C(71)	116.9(4)	C(31)	C(36)	C(35)	121.1(12)
Ir(2)	P(4)	C(81)	112.1(4)	P(2)	C(41)	C(42)	125.3(10)
C(6)	P(4)	C(71)	107.0(6)	P(2)	C(41)	C(46)	114.9(9)
C(6)	P(4)	C(81)	100.1(5)	C(42)	C(41)	C(46)	119.6(12)
C(71)	P(4)	C(81)	105.2(6)	C(41)	C(42)	C(43)	121.4(14)
P(1)	C(11)	C(12)	119.2(12)	C(42)	C(43)	C(44)	121.1(14)
P(1)	C(11)	C(16)	122.6(10)	C(43)	C(44)	C(45)	118.5(14)
C(12)	C(11)	C(16)	118.2(13)	C(44)	C(45)	C(46)	119.9(15)
C(11)	C(12)	C(13)	120.2(18)	C(41)	C(46)	C(45)	119.3(13)
C(12)	C(13)	C(14)	118.5(18)	P(3)	C(51)	C(52)	122.1(9)
C(13)	C(14)	C(15)	122.5(16)	P(3)	C(51)	C(56)	120.5(9)
C(14)	C(15)	C(16)	119.6(18)	C(52)	C(51)	C(56)	117.4(11)
C(11)	C(16)	C(15)	121.1(15)	C(51)	C(52)	C(53)	122.2(12)

Table S–4. Selected Interatomic Angles for Compound **4** (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C(52)	C(53)	C(54)	120.0(13)	C(72)	C(71)	C(76)	118.2(11)
C(53)	C(54)	C(55)	120.0(12)	C(71)	C(72)	C(73)	119.9(13)
C(54)	C(55)	C(56)	119.6(12)	C(72)	C(73)	C(74)	122.0(16)
C(51)	C(56)	C(55)	120.8(12)	C(73)	C(74)	C(75)	119.4(16)
P(3)	C(61)	C(62)	122.3(9)	C(74)	C(75)	C(76)	119.8(16)
P(3)	C(61)	C(66)	119.0(9)	C(71)	C(76)	C(75)	120.5(13)
C(62)	C(61)	C(66)	118.4(11)	P(4)	C(81)	C(82)	124.9(11)
C(61)	C(62)	C(63)	121.8(13)	P(4)	C(81)	C(86)	116.7(10)
C(62)	C(63)	C(64)	119.8(14)	C(82)	C(81)	C(86)	118.1(13)
C(63)	C(64)	C(65)	119.6(13)	C(81)	C(82)	C(83)	122.5(16)
C(64)	C(65)	C(66)	118.7(13)	C(82)	C(83)	C(84)	117.5(16)
C(61)	C(66)	C(65)	121.6(13)	C(83)	C(84)	C(85)	120.9(15)
P(4)	C(71)	C(72)	122.9(9)	C(84)	C(85)	C(86)	121.2(17)
P(4)	C(71)	C(76)	118.9(9)	C(81)	C(86)	C(85)	119.7(16)

(c) within the solvent dichloromethane molecule

Atom1	Atom2	Atom3	Angle
Cl(1)	C(91)	Cl(2)	114.1(12)

Table S–5. Anisotropic Displacement Parameters for Compound **4** (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir(1)	0.0293(3)	0.0279(3)	0.0322(3)	0.0003(2)	0.0121(2)	0.0012(2)
Ir(2)	0.0350(3)	0.0255(3)	0.0312(3)	-0.0003(2)	0.0122(2)	-0.0004(2)
I(1)	0.0329(5)	0.0749(6)	0.0488(5)	-0.0003(5)	0.0131(4)	-0.0121(4)
I(2)	0.065(5)	0.029(4)	0.041(5)	0.000(4)	0.010(4)	0.016(4)
P(1)	0.034(2)	0.0236(14)	0.034(2)	0.0003(12)	0.0131(13)	-0.0009(12)
P(2)	0.031(2)	0.0273(15)	0.034(2)	-0.0012(12)	0.0134(13)	-0.0016(12)
P(3)	0.031(2)	0.033(2)	0.029(2)	-0.0020(12)	0.0097(13)	-0.0007(13)
P(4)	0.032(2)	0.0269(15)	0.033(2)	0.0052(12)	0.0105(13)	0.0027(13)
O(1)	0.078(7)	0.065(6)	0.063(6)	0.001(5)	0.038(6)	0.034(6)
O(2)	0.044(6)	0.051(5)	0.047(5)	-0.004(4)	0.015(4)	-0.001(4)
O(3)	0.054(7)	0.027(6)	0.034(7)	-0.012(5)	0.013(6)	-0.006(5)
C(1)	0.047(8)	0.059(9)	0.031(7)	0.007(6)	0.012(6)	0.004(7)
C(2)	0.026(7)	0.055(8)	0.029(6)	0.008(6)	0.011(5)	0.001(6)
C(3)	0.052(11)	0.029(11)	0.049(14)	-0.017(8)	0.010(10)	-0.004(9)
C(4)	0.141(19)	0.025(9)	0.043(10)	-0.005(7)	0.017(11)	-0.004(10)
C(5)	0.036(7)	0.022(6)	0.042(7)	0.003(5)	0.014(6)	0.001(5)
C(6)	0.037(7)	0.036(7)	0.024(6)	0.003(5)	0.007(5)	0.006(5)
C(11)	0.064(9)	0.031(7)	0.031(7)	0.000(5)	0.017(6)	-0.006(6)
C(12)	0.106(14)	0.029(8)	0.085(12)	-0.008(8)	0.043(11)	0.003(8)
C(13)	0.156(21)	0.029(9)	0.081(13)	-0.009(8)	0.040(14)	-0.002(11)
C(14)	0.129(18)	0.029(9)	0.064(11)	0.013(8)	0.009(11)	-0.022(10)
C(15)	0.084(13)	0.052(10)	0.087(13)	0.005(9)	0.027(10)	-0.017(9)
C(16)	0.061(10)	0.036(8)	0.090(11)	0.001(7)	0.039(9)	-0.015(7)
C(21)	0.044(7)	0.029(6)	0.031(7)	0.002(5)	0.007(6)	0.006(5)
C(22)	0.060(9)	0.035(7)	0.049(8)	-0.002(6)	0.019(7)	0.004(6)
C(23)	0.060(10)	0.056(9)	0.055(9)	0.009(7)	0.020(8)	0.013(8)
C(24)	0.035(8)	0.058(9)	0.064(10)	0.009(8)	0.003(7)	0.010(7)
C(25)	0.039(8)	0.048(8)	0.074(11)	0.008(8)	0.012(7)	-0.005(7)
C(26)	0.032(7)	0.040(7)	0.062(9)	0.012(6)	0.017(6)	0.002(6)
C(31)	0.035(6)	0.035(6)	0.027(6)	0.001(5)	0.010(5)	0.011(5)
C(32)	0.036(7)	0.047(7)	0.026(6)	0.008(5)	0.010(5)	-0.002(6)
C(33)	0.048(8)	0.047(8)	0.062(9)	-0.002(7)	0.018(7)	-0.008(7)
C(34)	0.054(9)	0.058(9)	0.042(8)	0.003(7)	0.007(7)	-0.007(7)
C(35)	0.071(10)	0.048(8)	0.037(7)	0.016(6)	0.016(7)	0.016(8)
C(36)	0.041(7)	0.039(7)	0.042(7)	-0.003(6)	0.017(6)	0.004(6)
C(41)	0.040(7)	0.035(7)	0.053(8)	0.000(6)	0.032(6)	0.000(6)
C(42)	0.052(8)	0.041(7)	0.057(9)	-0.014(7)	0.028(7)	-0.004(6)
C(43)	0.083(13)	0.054(9)	0.083(12)	-0.017(8)	0.055(11)	0.009(9)

Table S–5. Anisotropic Displacement Parameters for Compound **4** (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(44)	0.066(11)	0.077(11)	0.106(14)	-0.015(11)	0.054(11)	0.014(9)
C(45)	0.039(8)	0.076(11)	0.096(13)	-0.016(10)	0.020(9)	0.002(8)
C(46)	0.046(8)	0.066(9)	0.056(9)	-0.008(7)	0.023(7)	0.005(7)
C(51)	0.029(6)	0.037(7)	0.049(7)	0.011(6)	0.021(6)	0.005(5)
C(52)	0.039(7)	0.056(8)	0.036(7)	-0.008(6)	0.013(6)	-0.004(6)
C(53)	0.033(7)	0.074(10)	0.060(9)	-0.009(8)	0.020(7)	-0.012(7)
C(54)	0.049(8)	0.049(8)	0.056(9)	-0.005(7)	0.030(7)	-0.004(7)
C(55)	0.052(8)	0.057(8)	0.033(7)	0.009(6)	0.022(6)	0.005(7)
C(56)	0.048(8)	0.048(8)	0.044(8)	-0.003(6)	0.021(6)	-0.002(6)
C(61)	0.028(6)	0.046(7)	0.022(6)	-0.003(5)	0.008(5)	-0.006(5)
C(62)	0.049(8)	0.040(7)	0.039(7)	-0.012(6)	0.016(6)	-0.005(6)
C(63)	0.047(9)	0.074(11)	0.048(8)	-0.012(8)	0.012(7)	-0.005(8)
C(64)	0.047(8)	0.063(10)	0.056(9)	-0.024(8)	0.009(7)	-0.016(7)
C(65)	0.058(9)	0.043(8)	0.068(10)	-0.014(7)	0.015(8)	0.005(7)
C(66)	0.049(8)	0.042(8)	0.044(8)	-0.011(6)	0.008(6)	0.004(6)
C(71)	0.032(7)	0.030(6)	0.042(7)	0.007(5)	0.013(6)	0.001(5)
C(72)	0.046(8)	0.054(8)	0.047(8)	0.010(7)	0.017(7)	0.001(7)
C(73)	0.074(12)	0.083(12)	0.072(11)	0.027(10)	0.036(10)	-0.006(10)
C(74)	0.067(12)	0.097(15)	0.117(17)	0.044(13)	0.024(12)	-0.030(11)
C(75)	0.070(12)	0.117(16)	0.088(14)	0.032(12)	-0.007(10)	-0.054(12)
C(76)	0.059(9)	0.063(9)	0.048(8)	0.017(7)	0.007(7)	-0.036(8)
C(81)	0.051(8)	0.032(7)	0.023(6)	-0.002(5)	0.008(6)	0.013(6)
C(82)	0.056(9)	0.049(8)	0.046(8)	0.004(6)	0.014(7)	0.017(7)
C(83)	0.088(13)	0.064(10)	0.057(10)	0.005(8)	0.021(9)	0.038(10)
C(84)	0.064(11)	0.090(13)	0.047(9)	0.009(9)	0.013(8)	0.039(10)
C(85)	0.033(8)	0.138(18)	0.069(11)	-0.010(12)	0.018(8)	0.005(10)
C(86)	0.031(7)	0.073(10)	0.062(9)	-0.006(8)	0.015(7)	-0.005(7)
Cl(1)	0.095(4)	0.099(4)	0.163(6)	-0.047(4)	-0.001(4)	-0.017(3)
Cl(2)	0.230(10)	0.104(5)	0.200(8)	0.009(5)	0.083(8)	-0.037(6)
C(91)	0.115(19)	0.095(16)	0.120(19)	-0.033(15)	-0.023(15)	0.010(14)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table S–6. Derived Parameters for Hydrogen Atoms of Compound **4**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(3A)[a]	0.3103	-0.1683	-0.1107	0.055
H(3B)[a]	0.2480	-0.2187	-0.0946	0.055
H(4A)[a]	0.2109	-0.2672	-0.2642	0.091
H(4B)[a]	0.2315	-0.3163	-0.1908	0.091
H(4C)[a]	0.2904	-0.2573	-0.2073	0.091
H(5A)	0.3018	0.1750	-0.1465	0.041
H(5B)	0.2339	0.1934	-0.2161	0.041
H(6A)	0.3054	-0.0764	0.1397	0.041
H(6B)	0.3569	-0.0279	0.1077	0.041
H(12)	0.1484	0.3963	-0.0960	0.086
H(13)	0.1913	0.5567	-0.0760	0.108
H(14)	0.2967	0.5942	-0.0874	0.099
H(15)	0.3634	0.4814	-0.1149	0.092
H(16)	0.3271	0.3231	-0.1274	0.071
H(22)	0.1289	0.2853	-0.2605	0.058
H(23)	0.0086	0.3008	-0.3375	0.069
H(24)	-0.0824	0.2574	-0.3015	0.068
H(25)	-0.0574	0.2064	-0.1921	0.068
H(26)	0.0624	0.1832	-0.1155	0.054
H(32)	0.0942	-0.0488	-0.2131	0.044
H(33)	-0.0130	-0.0542	-0.3109	0.064
H(34)	-0.0221	0.0171	-0.4122	0.066
H(35)	0.0775	0.0932	-0.4196	0.064
H(36)	0.1849	0.0996	-0.3241	0.049
H(42)	0.2531	-0.0614	-0.2984	0.057
H(43)	0.3513	-0.1069	-0.3206	0.080
H(44)	0.4688	-0.0815	-0.2389	0.092
H(45)	0.4842	-0.0113	-0.1323	0.087
H(46)	0.3819	0.0384	-0.1112	0.066
H(52)	0.1007	0.0718	0.0292	0.053
H(53)	0.0093	0.0404	0.0653	0.066
H(54)	0.0353	-0.0117	0.1779	0.058
H(55)	0.1549	-0.0291	0.2545	0.055
H(56)	0.2482	0.0095	0.2188	0.055
H(62)	0.3779	0.0330	0.2213	0.051
H(63)	0.4511	0.1237	0.3160	0.070
H(64)	0.4399	0.2878	0.3138	0.071
H(65)	0.3535	0.3637	0.2142	0.071
H(66)	0.2758	0.2690	0.1253	0.058
H(72)	0.2472	-0.2224	0.1359	0.059
H(73)	0.1555	-0.3147	0.1435	0.088
H(74)	0.0495	-0.3329	0.0525	0.117
H(75)	0.0366	-0.2727	-0.0546	0.124
H(76)	0.1274	-0.1765	-0.0645	0.073
H(82)	0.2985	-0.3228	0.0518	0.062
H(83)	0.3952	-0.4240	0.0624	0.086
H(84)	0.4964	-0.3578	0.0500	0.084
H(85)	0.5044	-0.1953	0.0372	0.096
H(86)	0.4092	-0.0962	0.0256	0.067
H(91A)	0.5232	0.7275	-0.1529	0.157
H(91B)	0.4494	0.7354	-0.1425	0.157

Table S–6. Derived Parameters for Hydrogen Atoms of Compound **4** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2

[a]Included with an occupancy factor of 0.85.

Table S–7. Crystallographic Experimental Details for Compound **10**.

A. Crystal Data	
formula	$C_{57}H_{51}IIr_2O_4P_4$
formula weight	1435.16
crystal dimensions (mm)	0.42 × 0.24 × 0.03
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	12.905 (2)
b (Å)	18.492 (3)
c (Å)	11.963 (2)
α (deg)	97.020 (14)
β (deg)	113.434 (12)
γ (deg)	78.438 (12)
V (Å^3)	2563.5 (7)
Z	2
ρ_{calcd} (g cm^{-3})	1.859
μ (mm^{-1})	5.960
B. Data Collection and Refinement Conditions	
diffractometer	Enraf-Nonius CAD4[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–50
scan type	θ–2θ
data collection 2θ limit (deg)	50.0
total data collected	9403 ($0 \le h \le 15$, $-21 \le k \le 21$, $-14 \le l \le 13$)
independent reflections	8964
number of observations (*NO*)	4784 ($F_o^2 \ge 2\sigma(F_o^2)$)
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	*DIFABS*[e]
range of transmission factors	1.255–0.844
data/restraints/parameters	8961/0/563
goodness-of-fit (S)[f]	1.015 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[g]	
$F_o^2 > 2\sigma(F_o^2)$	$\boldsymbol{R_1 = 0.0622}$, $wR_2 = 0.1270$
all data	$R_1 = 0.1784$, $\boldsymbol{wR_2 = 0.1646}$
largest difference peak and hole	1.782 and –1.820 e Å^{-3}

(continued)

Table S–7. Crystallographic Experimental Details for Compound **10** (continued)

[a]Obtained from least-squares refinement of 24 reflections with $20.1° < 2\theta < 23.8°$.

[b]Programs for diffractometer operation and data collection were those supplied by Enraf-Nonius.

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections except for 3 having $F_o^2 < -3\sigma(F_o^2)$. Weighted R-factors wR_2 and all goodnesses of fit S are based on F_o^2; conventional R-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. R-factors based on F_o^2 are statistically about twice as large as those based on F_o, and R-factors based on ALL data will be even larger.

[e]Walker, N.; Stuart, D. *Acta Crystallogr.* **1983**, *A39*, 158–166.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0608P)^2 + 0.9018P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S–8. Atomic Coordinates and Displacement Parameters for Compound **10**.

(a) 'inner-sphere' atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ir(1)	0.23861(6)	0.23926(4)	0.04195(7)	0.0205(2)*
Ir(2)	0.23053(6)	0.29577(4)	0.26540(7)	0.0186(2)*
I	0.26489(11)	0.14062(7)	0.21828(12)	0.0271(3)*
P(1)	0.0404(5)	0.2377(3)	-0.0467(5)	0.0254(13)*
P(2)	0.0333(4)	0.2937(3)	0.1976(5)	0.0207(12)*
P(3)	0.4382(4)	0.2282(3)	0.1152(4)	0.0195(11)*
P(4)	0.4255(4)	0.2999(3)	0.3512(5)	0.0204(12)*
O(1)	0.2361(14)	0.2272(9)	-0.2108(14)	0.056(5)*
O(2)	0.1849(13)	0.4048(7)	0.0773(13)	0.038(4)*
O(3)	0.2164(12)	0.3959(8)	0.4759(14)	0.051(4)*
C(1)	0.2398(19)	0.2271(12)	-0.1130(21)	0.044(6)*
C(2)	0.2098(14)	0.3443(10)	0.1113(16)	0.022(4)*
C(3)	0.2194(15)	0.3562(10)	0.3958(17)	0.026(4)*
C(4)	-0.0342(17)	0.2747(10)	0.0438(17)	0.030(5)*
C(5)	0.5051(15)	0.2312(9)	0.2808(16)	0.020(4)*

(b) dppm phenyl carbons

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(11)	0.0094(17)	0.1463(11)	-0.1056(19)	0.032(5)*
C(12)	-0.0754(18)	0.1179(12)	-0.0863(17)	0.037(6)*
C(13)	-0.0976(23)	0.0476(13)	-0.1276(21)	0.057(7)*
C(14)	-0.0408(21)	0.0037(13)	-0.1869(23)	0.061(8)*
C(15)	0.0426(21)	0.0295(14)	-0.2108(24)	0.064(8)*
C(16)	0.0684(19)	0.0988(11)	-0.1662(22)	0.050(7)*
C(21)	-0.0314(17)	0.2909(11)	-0.1871(17)	0.031(5)*
C(22)	-0.0448(18)	0.3666(12)	-0.1706(20)	0.042(6)*
C(23)	-0.0944(18)	0.4089(13)	-0.2681(22)	0.047(6)*
C(24)	-0.1372(20)	0.3798(14)	-0.3835(24)	0.054(7)*
C(25)	-0.1256(20)	0.3047(15)	-0.4044(22)	0.055(7)*
C(26)	-0.0710(19)	0.2611(13)	-0.3059(20)	0.048(6)*
C(31)	0.0048(14)	0.2339(9)	0.2903(16)	0.017(4)
C(32)	0.0782(17)	0.2188(11)	0.4125(20)	0.039(6)*
C(33)	0.0492(16)	0.1740(10)	0.4775(18)	0.032(5)*
C(34)	-0.0503(17)	0.1467(11)	0.4253(19)	0.036(5)
C(35)	-0.1207(18)	0.1591(10)	0.3075(19)	0.035(5)*
C(36)	-0.0925(16)	0.2017(10)	0.2391(19)	0.035(5)*
C(41)	-0.0428(15)	0.3827(10)	0.2326(17)	0.025(5)*
C(42)	-0.0548(15)	0.4036(10)	0.3419(17)	0.024(4)
C(43)	-0.1074(16)	0.4726(10)	0.3651(19)	0.030(5)*
C(44)	-0.1505(15)	0.5225(10)	0.2767(20)	0.034(5)*
C(45)	-0.1451(19)	0.5052(12)	0.1630(20)	0.045(6)*
C(46)	-0.0907(16)	0.4357(10)	0.1420(18)	0.027(5)*
C(51)	0.5166(15)	0.1431(9)	0.0750(16)	0.017(4)
C(52)	0.5235(22)	0.1389(12)	-0.0397(23)	0.054(7)*
C(53)	0.5877(23)	0.0785(16)	-0.0787(25)	0.068(8)*
C(54)	0.6386(21)	0.0229(14)	-0.0062(23)	0.053(7)*
C(55)	0.6327(18)	0.0255(12)	0.1100(20)	0.042(6)*
C(56)	0.5699(17)	0.0851(11)	0.1446(19)	0.035(5)*
C(61)	0.4895(15)	0.2977(9)	0.0648(16)	0.019(4)*
C(62)	0.4189(15)	0.3529(10)	-0.0086(18)	0.029(5)*
C(63)	0.4617(18)	0.4032(10)	-0.0472(18)	0.032(5)*

Table S–8. Atomic Coordinates and Displacement Parameters for Compound **10** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(64)	0.5796(20)	0.3999(12)	-0.0063(21)	0.043(6)*
C(65)	0.6499(21)	0.3470(12)	0.0695(21)	0.048(6)*
C(66)	0.6082(14)	0.2958(10)	0.1051(16)	0.024(4)*
C(71)	0.4923(15)	0.2770(9)	0.5122(14)	0.016(4)*
C(72)	0.5969(16)	0.2952(10)	0.5895(17)	0.030(5)*
C(73)	0.6488(18)	0.2758(13)	0.7072(18)	0.047(6)*
C(74)	0.5949(21)	0.2380(12)	0.7514(20)	0.049(7)*
C(75)	0.4914(20)	0.2183(12)	0.6812(21)	0.049(6)
C(76)	0.4434(21)	0.2396(13)	0.5598(19)	0.058(8)*
C(81)	0.4649(15)	0.3869(10)	0.3415(16)	0.023(4)*
C(82)	0.3851(17)	0.4522(9)	0.3277(17)	0.029(5)*
C(83)	0.4080(18)	0.5198(11)	0.3194(20)	0.041(6)*
C(84)	0.5176(18)	0.5205(12)	0.3236(17)	0.035(5)*
C(85)	0.5979(16)	0.4597(12)	0.3376(19)	0.039(6)*
C(86)	0.5692(18)	0.3926(10)	0.3429(19)	0.036(5)*

(c) solvent tetrahydrofuran atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
O(90)	0.7444(29)	0.0727(20)	0.4536(32)	0.181(13)
C(91)	0.7131(36)	0.0925(23)	0.5400(40)	0.145(17)
C(92)	0.6306(36)	0.0447(23)	0.5317(39)	0.148(17)
C(93)	0.6646(36)	-0.0247(24)	0.4608(39)	0.151(17)
C(94)	0.7700(34)	-0.0041(23)	0.4548(37)	0.136(15)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table S–9. Selected Interatomic Distances for Compound **10** (Å)

(a) involving 'inner-sphere' atoms

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ir(1)	Ir(2)	2.7828(11)	Ir(2)	C(2)	2.05(2)
Ir(1)	I	2.831(2)	Ir(2)	C(3)	1.84(2)
Ir(1)	P(1)	2.352(5)	P(1)	C(4)	1.72(2)
Ir(1)	P(3)	2.341(5)	P(2)	C(4)	1.72(2)
Ir(1)	C(1)	1.85(2)	P(3)	C(5)	1.82(2)
Ir(1)	C(2)	2.04(2)	P(4)	C(5)	1.81(2)
Ir(2)	I	2.835(2)	O(1)	C(1)	1.15(2)
Ir(2)	P(2)	2.351(5)	O(2)	C(2)	1.18(2)
Ir(2)	P(4)	2.323(5)	O(3)	C(3)	1.14(2)

(b) involving dppm phenyl carbons

Atom1	Atom2	Distance	Atom1	Atom2	Distance
P(1)	C(11)	1.81(2)	C(42)	C(43)	1.37(2)
P(1)	C(21)	1.86(2)	C(43)	C(44)	1.36(2)
P(2)	C(31)	1.84(2)	C(44)	C(45)	1.39(3)
P(2)	C(41)	1.83(2)	C(45)	C(46)	1.38(3)
P(3)	C(51)	1.81(2)	C(51)	C(52)	1.40(3)
P(3)	C(61)	1.82(2)	C(51)	C(56)	1.34(2)
P(4)	C(71)	1.83(2)	C(52)	C(53)	1.40(3)
P(4)	C(81)	1.81(2)	C(53)	C(54)	1.32(3)
C(11)	C(12)	1.41(2)	C(54)	C(55)	1.42(3)
C(11)	C(16)	1.38(3)	C(55)	C(56)	1.36(3)
C(12)	C(13)	1.38(3)	C(61)	C(62)	1.36(2)
C(13)	C(14)	1.32(3)	C(61)	C(66)	1.41(2)
C(14)	C(15)	1.40(3)	C(62)	C(63)	1.38(2)
C(15)	C(16)	1.38(3)	C(63)	C(64)	1.39(3)
C(21)	C(22)	1.37(3)	C(64)	C(65)	1.35(3)
C(21)	C(26)	1.39(3)	C(65)	C(66)	1.36(2)
C(22)	C(23)	1.35(3)	C(71)	C(72)	1.38(2)
C(23)	C(24)	1.35(3)	C(71)	C(76)	1.33(3)
C(24)	C(25)	1.37(3)	C(72)	C(73)	1.36(2)
C(25)	C(26)	1.37(3)	C(73)	C(74)	1.35(3)
C(31)	C(32)	1.42(3)	C(74)	C(75)	1.36(3)
C(31)	C(36)	1.38(2)	C(75)	C(76)	1.40(3)
C(32)	C(33)	1.39(3)	C(81)	C(82)	1.40(2)
C(33)	C(34)	1.36(2)	C(81)	C(86)	1.36(3)
C(34)	C(35)	1.36(3)	C(82)	C(83)	1.37(2)
C(35)	C(36)	1.39(3)	C(83)	C(84)	1.40(3)
C(41)	C(42)	1.38(2)	C(84)	C(85)	1.34(3)
C(41)	C(46)	1.42(2)	C(85)	C(86)	1.38(2)

(c) within the solvent tetrahydrofuran molecule

Atom1	Atom2	Distance	Atom1	Atom2	Distance
O(90)	C(91)	1.24(5)	C(92)	C(93)	1.54(5)
O(90)	C(94)	1.39(4)	C(93)	C(94)	1.51(5)
C(91)	C(92)	1.48(4)			

Table S–10. Selected Interatomic Angles for Compound **10** (deg)

(a) involving 'inner-sphere' atoms

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ir(2)	Ir(1)	I	60.66(4)	I	Ir(2)	P(4)	93.24(13)
Ir(2)	Ir(1)	P(1)	92.76(14)	I	Ir(2)	C(2)	107.4(5)
Ir(2)	Ir(1)	P(3)	93.02(13)	I	Ir(2)	C(3)	134.4(6)
Ir(2)	Ir(1)	C(1)	165.2(7)	P(2)	Ir(2)	P(4)	174.5(2)
Ir(2)	Ir(1)	C(2)	47.2(5)	P(2)	Ir(2)	C(2)	92.2(5)
I	Ir(1)	P(1)	90.52(13)	P(2)	Ir(2)	C(3)	88.2(6)
I	Ir(1)	P(3)	89.04(12)	P(4)	Ir(2)	C(2)	92.3(5)
I	Ir(1)	C(1)	134.1(7)	P(4)	Ir(2)	C(3)	86.9(6)
I	Ir(1)	C(2)	107.8(5)	C(2)	Ir(2)	C(3)	118.2(8)
P(1)	Ir(1)	P(3)	173.1(2)	Ir(1)	I	Ir(2)	58.83(3)
P(1)	Ir(1)	C(1)	88.2(7)	Ir(1)	P(1)	C(4)	115.4(7)
P(1)	Ir(1)	C(2)	90.4(5)	Ir(2)	P(2)	C(4)	115.2(7)
P(3)	Ir(1)	C(1)	87.1(7)	Ir(1)	P(3)	C(5)	112.9(6)
P(3)	Ir(1)	C(2)	96.2(5)	Ir(2)	P(4)	C(5)	112.2(6)
C(1)	Ir(1)	C(2)	118.1(8)	Ir(1)	C(1)	O(1)	173.0(22)
Ir(1)	Ir(2)	I	60.51(4)	Ir(1)	C(2)	Ir(2)	85.9(7)
Ir(1)	Ir(2)	P(2)	92.75(13)	Ir(1)	C(2)	O(2)	137.7(15)
Ir(1)	Ir(2)	P(4)	92.64(13)	Ir(2)	C(2)	O(2)	136.3(15)
Ir(1)	Ir(2)	C(2)	47.0(5)	Ir(2)	C(3)	O(3)	176.2(17)
Ir(1)	Ir(2)	C(3)	165.1(6)	P(1)	C(4)	P(2)	122.2(12)
I	Ir(2)	P(2)	88.42(13)	P(3)	C(5)	P(4)	112.7(10)

(b) involving dppm phenyl carbons

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ir(1)	P(1)	C(11)	111.9(7)	P(1)	C(21)	C(22)	116.4(15)
Ir(1)	P(1)	C(21)	112.2(6)	P(1)	C(21)	C(26)	126.0(17)
C(4)	P(1)	C(11)	110.3(9)	C(22)	C(21)	C(26)	117.7(20)
C(4)	P(1)	C(21)	104.5(9)	C(21)	C(22)	C(23)	119.9(22)
C(11)	P(1)	C(21)	101.4(9)	C(22)	C(23)	C(24)	122.2(23)
Ir(2)	P(2)	C(31)	111.0(6)	C(23)	C(24)	C(25)	119.9(23)
Ir(2)	P(2)	C(41)	110.9(5)	C(24)	C(25)	C(26)	118.1(23)
C(4)	P(2)	C(31)	112.3(8)	C(21)	C(26)	C(25)	122.1(23)
C(4)	P(2)	C(41)	106.5(9)	P(2)	C(31)	C(32)	123.2(13)
C(31)	P(2)	C(41)	99.7(8)	P(2)	C(31)	C(36)	118.9(14)
Ir(1)	P(3)	C(51)	117.3(6)	C(32)	C(31)	C(36)	117.9(16)
Ir(1)	P(3)	C(61)	114.8(6)	C(31)	C(32)	C(33)	119.6(17)
C(5)	P(3)	C(51)	101.8(8)	C(32)	C(33)	C(34)	120.3(19)
C(5)	P(3)	C(61)	106.6(8)	C(33)	C(34)	C(35)	121.0(19)
C(51)	P(3)	C(61)	101.9(8)	C(34)	C(35)	C(36)	120.0(19)
Ir(2)	P(4)	C(71)	113.1(6)	C(31)	C(36)	C(35)	121.0(19)
Ir(2)	P(4)	C(81)	115.5(6)	P(2)	C(41)	C(42)	125.4(15)
C(5)	P(4)	C(71)	103.0(8)	P(2)	C(41)	C(46)	118.0(15)
C(5)	P(4)	C(81)	105.1(8)	C(42)	C(41)	C(46)	116.6(18)
C(71)	P(4)	C(81)	106.9(8)	C(41)	C(42)	C(43)	122.8(19)
P(1)	C(11)	C(12)	120.9(17)	C(42)	C(43)	C(44)	119.0(20)
P(1)	C(11)	C(16)	123.6(15)	C(43)	C(44)	C(45)	121.9(19)
C(12)	C(11)	C(16)	115.5(19)	C(44)	C(45)	C(46)	118.2(19)
C(11)	C(12)	C(13)	121.5(22)	C(41)	C(46)	C(45)	121.6(20)
C(12)	C(13)	C(14)	121.7(24)	P(3)	C(51)	C(52)	116.4(15)
C(13)	C(14)	C(15)	119.3(22)	P(3)	C(51)	C(56)	126.5(16)
C(14)	C(15)	C(16)	119.4(25)	C(52)	C(51)	C(56)	117.1(19)
C(11)	C(16)	C(15)	122.5(23)	C(51)	C(52)	C(53)	122.1(22)

Table S–10. Selected Interatomic Angles for Compound **10** (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C(52)	C(53)	C(54)	118.0(25)	C(72)	C(71)	C(76)	116.1(17)
C(53)	C(54)	C(55)	121.0(25)	C(71)	C(72)	C(73)	122.9(18)
C(54)	C(55)	C(56)	119.2(22)	C(72)	C(73)	C(74)	118.6(19)
C(51)	C(56)	C(55)	122.4(21)	C(73)	C(74)	C(75)	122.1(21)
P(3)	C(61)	C(62)	123.5(14)	C(74)	C(75)	C(76)	116.2(21)
P(3)	C(61)	C(66)	118.8(14)	C(71)	C(76)	C(75)	124.2(20)
C(62)	C(61)	C(66)	117.7(16)	P(4)	C(81)	C(82)	119.8(14)
C(61)	C(62)	C(63)	121.4(18)	P(4)	C(81)	C(86)	123.3(15)
C(62)	C(63)	C(64)	119.6(19)	C(82)	C(81)	C(86)	116.9(18)
C(63)	C(64)	C(65)	119.3(20)	C(81)	C(82)	C(83)	123.4(19)
C(64)	C(65)	C(66)	121.4(22)	C(82)	C(83)	C(84)	115.6(20)
C(61)	C(66)	C(65)	120.6(19)	C(83)	C(84)	C(85)	123.5(18)
P(4)	C(71)	C(72)	122.6(14)	C(84)	C(85)	C(86)	118.4(18)
P(4)	C(71)	C(76)	121.2(14)	C(81)	C(86)	C(85)	122.1(20)

(c) within the solvent tetrahydrofuran molecule

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C(91)	O(90)	C(94)	105.2(38)	C(92)	C(93)	C(94)	98.7(33)
O(90)	C(91)	C(92)	106.9(38)	O(90)	C(94)	C(93)	102.8(36)
C(91)	C(92)	C(93)	102.6(36)				

Table S–11. Anisotropic Displacement Parameters for Compound **10** (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir(1)	0.0193(5)	0.0234(5)	0.0191(5)	0.0009(4)	0.0072(4)	-0.0042(4)
Ir(2)	0.0188(5)	0.0184(5)	0.0184(5)	0.0004(3)	0.0071(4)	-0.0030(4)
I	0.0307(7)	0.0195(7)	0.0333(8)	0.0024(6)	0.0142(6)	-0.0046(6)
P(1)	0.027(3)	0.031(3)	0.019(3)	-0.005(2)	0.008(2)	-0.012(3)
P(2)	0.018(3)	0.021(3)	0.026(3)	0.004(2)	0.011(2)	-0.002(2)
P(3)	0.017(3)	0.024(3)	0.014(3)	0.004(2)	0.003(2)	-0.001(2)
P(4)	0.019(3)	0.020(3)	0.023(3)	0.002(2)	0.007(2)	-0.005(2)
O(1)	0.064(12)	0.095(14)	0.024(9)	-0.008(8)	0.023(8)	-0.040(10)
O(2)	0.063(11)	0.028(8)	0.034(9)	-0.003(7)	0.028(8)	-0.013(8)
O(3)	0.046(10)	0.063(11)	0.048(10)	-0.040(9)	0.024(8)	-0.029(9)
C(1)	0.047(15)	0.052(15)	0.046(16)	0.004(12)	0.027(13)	-0.023(12)
C(2)	0.009(9)	0.026(11)	0.022(11)	0.014(8)	-0.008(8)	-0.006(8)
C(3)	0.016(10)	0.031(11)	0.023(11)	-0.006(9)	0.005(9)	0.002(9)
C(4)	0.033(12)	0.036(12)	0.017(11)	-0.001(9)	0.011(9)	0.007(10)
C(5)	0.016(10)	0.014(10)	0.027(11)	0.002(8)	0.001(9)	-0.007(8)
C(11)	0.027(12)	0.034(12)	0.036(13)	0.014(10)	0.008(10)	-0.005(10)
C(12)	0.054(15)	0.053(14)	0.016(11)	-0.002(10)	0.017(10)	-0.032(12)
C(13)	0.088(21)	0.053(17)	0.045(16)	-0.017(13)	0.039(16)	-0.024(16)
C(14)	0.057(17)	0.041(15)	0.060(18)	-0.009(13)	-0.009(14)	-0.026(14)
C(15)	0.054(17)	0.050(17)	0.069(20)	-0.016(14)	0.013(15)	0.001(14)
C(16)	0.037(14)	0.029(13)	0.067(18)	-0.003(12)	0.003(13)	-0.011(11)
C(21)	0.032(12)	0.037(13)	0.020(11)	-0.004(9)	0.005(9)	-0.015(10)
C(22)	0.040(14)	0.050(15)	0.033(13)	0.013(11)	-0.001(11)	-0.025(12)
C(23)	0.033(14)	0.045(15)	0.047(16)	0.027(12)	0.002(12)	0.017(11)
C(24)	0.053(17)	0.058(17)	0.058(18)	0.030(14)	0.026(14)	0.000(14)
C(25)	0.044(16)	0.085(21)	0.036(16)	0.004(14)	0.018(13)	-0.003(15)
C(26)	0.057(16)	0.047(15)	0.031(14)	-0.011(11)	0.017(12)	0.005(13)
C(32)	0.027(12)	0.040(13)	0.047(15)	0.008(11)	0.007(11)	-0.012(10)
C(33)	0.031(12)	0.022(11)	0.033(13)	0.016(9)	0.003(10)	0.008(9)
C(35)	0.047(14)	0.027(12)	0.042(14)	0.006(10)	0.022(11)	-0.015(10)
C(36)	0.023(11)	0.025(11)	0.035(13)	0.009(9)	-0.005(10)	0.013(9)
C(41)	0.015(10)	0.033(12)	0.021(11)	0.003(9)	-0.003(8)	-0.013(9)
C(43)	0.027(12)	0.018(11)	0.038(13)	0.004(9)	0.004(10)	-0.003(9)
C(44)	0.017(11)	0.021(11)	0.063(16)	0.019(10)	0.018(11)	0.014(9)
C(45)	0.056(16)	0.040(14)	0.041(15)	0.023(11)	0.027(13)	0.018(12)
C(46)	0.024(11)	0.021(11)	0.032(12)	0.007(9)	0.007(9)	0.000(9)
C(52)	0.084(20)	0.025(13)	0.060(18)	0.005(11)	0.037(16)	-0.001(13)
C(53)	0.082(22)	0.072(20)	0.061(20)	0.032(16)	0.044(18)	0.016(17)
C(54)	0.067(18)	0.053(17)	0.065(18)	-0.027(14)	0.050(16)	-0.036(15)
C(55)	0.032(13)	0.047(15)	0.036(14)	0.010(11)	0.004(11)	0.001(11)
C(56)	0.028(12)	0.036(13)	0.036(13)	0.023(10)	0.007(10)	0.012(10)
C(61)	0.030(11)	0.015(9)	0.016(10)	0.001(8)	0.017(9)	0.006(8)
C(62)	0.015(10)	0.032(12)	0.044(13)	0.006(10)	0.015(10)	-0.005(9)
C(63)	0.048(14)	0.019(10)	0.040(13)	0.020(9)	0.028(11)	0.005(10)
C(64)	0.053(16)	0.035(13)	0.049(15)	0.007(11)	0.028(13)	-0.007(12)
C(65)	0.054(16)	0.047(15)	0.059(17)	-0.009(13)	0.028(14)	-0.032(13)
C(66)	0.010(9)	0.033(11)	0.022(11)	0.000(9)	0.000(8)	0.000(8)
C(71)	0.021(10)	0.012(9)	0.003(9)	0.001(7)	-0.005(8)	0.003(8)
C(72)	0.029(12)	0.025(11)	0.031(12)	0.020(9)	-0.002(9)	-0.009(9)
C(73)	0.024(12)	0.081(18)	0.021(12)	0.014(12)	-0.009(10)	-0.009(12)
C(74)	0.075(18)	0.041(14)	0.024(13)	0.025(11)	0.010(12)	-0.004(13)

Table S–11. Anisotropic Displacement Parameters for Compound **10** (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(76)	0.063(17)	0.075(18)	0.018(12)	0.024(12)	-0.021(11)	-0.034(15)
C(81)	0.025(11)	0.027(11)	0.018(11)	0.008(8)	0.014(9)	0.013(9)
C(82)	0.031(12)	0.013(10)	0.035(12)	0.002(8)	0.007(10)	-0.001(9)
C(83)	0.038(13)	0.019(11)	0.059(16)	-0.005(10)	0.015(12)	-0.004(10)
C(84)	0.045(14)	0.043(14)	0.023(11)	0.001(9)	0.009(10)	-0.031(12)
C(85)	0.009(10)	0.060(15)	0.051(15)	0.038(12)	0.009(10)	0.003(10)
C(86)	0.045(14)	0.014(10)	0.064(16)	0.015(10)	0.031(12)	-0.005(10)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table S–12. Derived Parameters for Hydrogen Atoms of Compound **10**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(4)	-0.1146	0.2850	0.0080	0.037
H(5A)	0.5115	0.1825	0.3096	0.025
H(5B)	0.5827	0.2421	0.3063	0.025
H(12)	-0.1177	0.1477	-0.0443	0.045
H(13)	-0.1548	0.0305	-0.1130	0.069
H(14)	-0.0562	-0.0445	-0.2128	0.073
H(15)	0.0809	-0.0002	-0.2569	0.077
H(16)	0.1285	0.1142	-0.1776	0.060
H(22)	-0.0193	0.3887	-0.0915	0.051
H(23)	-0.0996	0.4605	-0.2556	0.057
H(24)	-0.1748	0.4110	-0.4493	0.065
H(25)	-0.1543	0.2836	-0.4841	0.066
H(26)	-0.0600	0.2095	-0.3192	0.058
H(32)	0.1461	0.2389	0.4497	0.047
H(33)	0.0988	0.1627	0.5579	0.039
H(34)	-0.0708	0.1186	0.4714	0.044
H(35)	-0.1886	0.1389	0.2722	0.042
H(36)	-0.1403	0.2087	0.1567	0.042
H(42)	-0.0258	0.3692	0.4031	0.029
H(43)	-0.1135	0.4852	0.4410	0.037
H(44)	-0.1850	0.5702	0.2932	0.040
H(45)	-0.1776	0.5398	0.1018	0.054
H(46)	-0.0852	0.4234	0.0657	0.032
H(52)	0.4837	0.1780	-0.0922	0.065
H(53)	0.5943	0.0776	-0.1544	0.082
H(54)	0.6794	-0.0192	-0.0320	0.063
H(55)	0.6718	-0.0136	0.1624	0.050
H(56)	0.5636	0.0855	0.2203	0.043
H(62)	0.3392	0.3567	-0.0336	0.035
H(63)	0.4115	0.4396	-0.1009	0.039
H(64)	0.6097	0.4343	-0.0313	0.051
H(65)	0.7296	0.3453	0.0985	0.058
H(66)	0.6592	0.2589	0.1571	0.029
H(72)	0.6337	0.3222	0.5592	0.036
H(73)	0.7208	0.2884	0.7570	0.056
H(74)	0.6301	0.2249	0.8333	0.058
H(75)	0.4541	0.1921	0.7121	0.059
H(76)	0.3721	0.2264	0.5091	0.070
H(82)	0.3119	0.4492	0.3240	0.034
H(83)	0.3535	0.5631	0.3113	0.049
H(84)	0.5362	0.5658	0.3163	0.042
H(85)	0.6717	0.4628	0.3436	0.047
H(86)	0.6233	0.3494	0.3476	0.044
H(91A)	0.6765	0.1445	0.5343	0.174
H(91B)	0.7790	0.0867	0.6179	0.174
H(92A)	0.5515	0.0682	0.4874	0.177
H(92B)	0.6389	0.0329	0.6128	0.177
H(93A)	0.6830	-0.0696	0.5055	0.181
H(93B)	0.6052	-0.0307	0.3795	0.181
H(94A)	0.8388	-0.0204	0.5262	0.163
H(94B)	0.7814	-0.0255	0.3806	0.163