Table S-1. Crystallographic Experimental Details for **2**

A. Crystal Data	
formula	$C_{81}H_{72}IrO_4P_4Ru$
formula weight	1526.54
crystal dimensions (mm)	0.36 × 0.28 × 0.26
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	14.0744 (6)
b (Å)	15.4510 (7)
c (Å)	17.6510 (8)
α (deg)	89.8086 (8)
β (deg)	70.6204 (8)
γ (deg)	74.9795 (7)
V (Å^3)	3482.8 (3)
Z	2
ρ_{calcd} (g cm^{-3})	1.456
μ (mm^{-1})	2.267
B. Data Collection and Refinement Conditions	
diffractometer	Bruker P4/RA/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ϕ rotations (0.3°) / ω scans (0.3°) (30 s exposures)
data collection 2θ limit (deg)	51.40
total data collected	18825 (-16 ≤ h ≤ 17, -18 ≤ k ≤ 18, -21 ≤ l ≤ 20)
independent reflections	13178
number of observations (*NO*)	11250 [$F_o^2 \geq 2\sigma(F_o^2)$]
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	0.6416–0.4104
data/restraints/parameters	13178 [$F_o^2 \geq -3\sigma(F_o^2)$] / 9[e] / 792
goodness-of-fit (S)[f]	1.040 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0365
wR_2 [$F_o^2 \geq -3\sigma(F_o^2)$]	0.0973
largest difference peak and hole	1.744 and –1.097 e Å^{-3}

[a]Obtained from least-squares refinement of 6209 centered reflections.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

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

(continued...)

Table S-1. Crystallographic Experimental Details for **2** (continued)

[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]The Ir–H(1) and Ir'–H(1') distances were fixed at 1.75 Å. Restraints were also applied to fix the geometries of the carbonyl ligand C(3')O(3') (d(Ir'–C(3')) = 1.92 Å; d(C(3')–O(3')) = 1.15 Å; d(Ir'···O(3')) = 3.07 Å) and the hydride ligand H(1') (d(P(2)···H(1')) = d(P(4)···H(1')) = 2.75 Å; d(C(2)···H(1')) = d(C(4)···H(1')) = 3.00 Å).

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0494P)^2 + 1.1045P]^{-1}$ where $P = [\text{Max}(F_o^2, 0) + 2F_c^2]/3$).

[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-2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **2**

(a) 'inner-core' atoms of [IrRuH(CO)$_3$(μ–CO)(dppm)$_2$]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ir/Ru'[a]	0.023099(13)	0.241421(11)	0.238369(10)	0.02526(6)*
Ru/Ir'[a]	-0.14543(2)	0.397699(18)	0.288162(16)	0.02805(8)*
P(1)	0.14900(8)	0.31612(7)	0.22461(6)	0.0262(2)*
P(2)	-0.03127(8)	0.48554(7)	0.28255(6)	0.0241(2)*
P(3)	-0.07828(8)	0.15023(7)	0.22501(6)	0.0265(2)*
P(4)	-0.26556(8)	0.31650(7)	0.29217(6)	0.0255(2)*
O(1)	0.0319(3)	0.1947(2)	0.4042(2)	0.0571(9)*
O(2)	-0.0408(2)	0.3410(2)	0.10527(17)	0.0362(7)*
O(3)[b]	-0.3000(3)	0.5597(3)	0.2531(3)	0.0500(10)*
O(3')[c]	0.1868(14)	0.1151(11)	0.0939(9)	0.072(7)*
O(4)	-0.1852(3)	0.3899(3)	0.4693(2)	0.0583(10)*
C(1)	0.0290(3)	0.2074(3)	0.3427(3)	0.0292(8)*
C(2)	-0.0477(3)	0.3311(2)	0.1735(2)	0.0265(8)*
C(3)[b]	-0.2412(4)	0.4996(3)	0.2656(3)	0.0314(11)*
C(3')[c]	0.1260(17)	0.1647(12)	0.1467(9)	0.040(7)
C(4)	-0.1725(3)	0.3928(3)	0.4039(2)	0.0320(9)*
C(5)	0.0948(3)	0.4216(3)	0.2899(2)	0.0270(8)*
C(6)	-0.2129(3)	0.1942(3)	0.2945(2)	0.0268(8)*
H(1)[b]	0.1282	0.1607	0.1703	0.050
H(1')[c]	-0.2302	0.4915	0.2672	0.050

(b) dppm phenyl carbons

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(11)	0.2564(3)	0.2558(3)	0.2577(3)	0.0314(9)*
C(12)	0.3125(4)	0.1686(3)	0.2216(3)	0.0447(11)*
C(13)	0.3923(4)	0.1189(3)	0.2453(4)	0.0542(13)*
C(14)	0.4166(4)	0.1522(4)	0.3065(3)	0.0526(14)*
C(15)	0.3626(4)	0.2371(4)	0.3424(3)	0.0494(12)*
C(16)	0.2829(3)	0.2890(3)	0.3182(3)	0.0394(10)*
C(21)	0.2180(3)	0.3490(3)	0.1259(2)	0.0308(9)*
C(22)	0.2001(4)	0.3265(4)	0.0573(3)	0.0515(13)*
C(23)	0.2495(5)	0.3576(5)	-0.0157(3)	0.0735(19)*
C(24)	0.3190(4)	0.4066(4)	-0.0207(3)	0.0609(15)*
C(25)	0.3381(4)	0.4279(4)	0.0457(3)	0.0557(14)*
C(26)	0.2882(4)	0.3999(3)	0.1200(3)	0.0451(11)*
C(31)	0.0067(3)	0.5498(3)	0.1957(2)	0.0276(8)*
C(32)	-0.0284(3)	0.5438(3)	0.1315(2)	0.0340(9)*
C(33)	-0.0002(4)	0.5942(3)	0.0658(3)	0.0420(11)*
C(34)	0.0615(4)	0.6512(3)	0.0657(3)	0.0413(11)*
C(35)	0.0958(4)	0.6575(3)	0.1299(3)	0.0457(12)*
C(36)	0.0687(4)	0.6073(3)	0.1939(3)	0.0414(11)*
C(41)	-0.0752(3)	0.5756(3)	0.3638(2)	0.0290(8)*
C(42)	-0.1622(4)	0.6455(3)	0.3691(3)	0.0491(12)*
C(43)	-0.1947(4)	0.7195(3)	0.4247(3)	0.0556(14)*
C(44)	-0.1418(4)	0.7247(3)	0.4767(3)	0.0465(12)*
C(45)	-0.0563(4)	0.6562(3)	0.4727(3)	0.0512(13)*
C(46)	-0.0236(4)	0.5810(3)	0.4174(3)	0.0418(11)*
C(51)	-0.0445(3)	0.0342(3)	0.2535(3)	0.0334(9)*
C(52)	0.0415(4)	0.0018(3)	0.2765(3)	0.0420(11)*
C(53)	0.0629(4)	-0.0851(3)	0.3018(3)	0.0523(13)*
C(54)	-0.0017(4)	-0.1385(3)	0.3024(4)	0.0562(14)*
C(55)	-0.0866(5)	-0.1073(3)	0.2774(4)	0.0634(16)*
C(56)	-0.1086(4)	-0.0213(3)	0.2531(4)	0.0540(14)*

Table S-2. Atomic Coordinates and Displacement Parameters for **2** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(61)	-0.0885(3)	0.1346(3)	0.1259(3)	0.0340(9)*
C(62)	-0.0032(4)	0.1327(3)	0.0559(3)	0.0473(12)*
C(63)	-0.0081(5)	0.1177(4)	-0.0196(3)	0.0605(16)*
C(64)	-0.0982(6)	0.1072(4)	-0.0278(3)	0.0631(16)*
C(65)	-0.1828(5)	0.1097(4)	0.0388(4)	0.0602(15)*
C(66)	-0.1787(4)	0.1227(3)	0.1155(3)	0.0440(11)*
C(71)	-0.3210(3)	0.3221(3)	0.2111(2)	0.0296(8)*
C(72)	-0.2821(3)	0.3620(3)	0.1408(3)	0.0376(10)*
C(73)	-0.3215(4)	0.3597(4)	0.0794(3)	0.0470(12)*
C(74)	-0.4016(4)	0.3198(4)	0.0864(3)	0.0482(12)*
C(75)	-0.4422(4)	0.2817(3)	0.1566(3)	0.0439(11)*
C(76)	-0.4022(3)	0.2825(3)	0.2181(3)	0.0373(10)*
C(81)	-0.3857(3)	0.3453(3)	0.3813(2)	0.0324(9)*
C(82)	-0.4640(4)	0.4226(3)	0.3824(3)	0.0457(11)*
C(83)	-0.5563(4)	0.4478(4)	0.4480(3)	0.0543(13)*
C(84)	-0.5701(4)	0.3988(4)	0.5132(3)	0.0637(17)*
C(85)	-0.4930(5)	0.3231(4)	0.5133(3)	0.0699(18)*
C(86)	-0.4011(4)	0.2966(4)	0.4467(3)	0.0516(13)*

(c) solvent benzene atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(11S)	-0.1386(6)	0.0767(5)	0.4980(4)	0.079(2)*
C(12S)	-0.1496(6)	-0.0036(5)	0.5275(4)	0.0778(19)*
C(13S)	-0.2291(6)	-0.0053(5)	0.5961(5)	0.082(2)*
C(14S)	-0.3010(6)	0.0713(6)	0.6343(5)	0.088(2)*
C(15S)	-0.2915(7)	0.1547(6)	0.6059(6)	0.099(3)*
C(16S)	-0.2071(7)	0.1557(5)	0.5361(5)	0.085(2)*
C(21S)	0.2806(7)	-0.3159(5)	0.2384(6)	0.090(2)*
C(22S)	0.2403(6)	-0.3511(6)	0.3077(5)	0.083(2)*
C(23S)	0.2829(6)	-0.4351(5)	0.3216(4)	0.0751(18)*
C(24S)	0.3703(6)	-0.4863(5)	0.2662(5)	0.0729(18)*
C(25S)	0.4161(5)	-0.4547(5)	0.1955(5)	0.085(2)*
C(26S)	0.3704(7)	-0.3670(6)	0.1811(5)	0.095(2)*
C(31S)	0.3516(6)	0.0442(7)	-0.2106(8)	0.121(4)*
C(32S)	0.2738(8)	0.0917(6)	-0.1444(6)	0.107(3)*
C(33S)	0.2307(8)	0.1838(5)	-0.1420(6)	0.102(3)*
C(34S)	0.2703(8)	0.2283(6)	-0.2079(5)	0.109(3)*
C(35S)	0.3523(9)	0.1809(7)	-0.2750(6)	0.115(3)*
C(36S)	0.3895(7)	0.0896(7)	-0.2764(7)	0.111(3)*
C(41S)[d]	-0.3343(7)	0.0289(5)	-0.0595(7)	0.183(2)
C(42S)[d]	-0.3265(7)	0.0642(7)	-0.1332(5)	0.183(2)
C(43S)[d]	-0.4063(9)	0.1360(7)	-0.1390(5)	0.183(2)
C(44S)[d]	-0.4938(7)	0.1724(5)	-0.0713(7)	0.183(2)
C(45S)[d]	-0.5016(6)	0.1370(7)	0.0024(5)	0.183(2)
C(46S)[d]	-0.4218(9)	0.0653(7)	0.0082(5)	0.183(2)
C(51S)	-0.4020(7)	-0.0451(5)	0.4968(7)	0.117(3)*
C(52S)	-0.4233(7)	0.0419(5)	0.4888(5)	0.096(3)*
C(53S)	-0.5173(8)	0.0886(5)	0.4873(6)	0.106(3)*

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]The metal atom positions were refined with the following partial occupancies in Ir and Ru: Ir/Ru', 0.833 Ir/0.167 Ru; Ru/Ir', 0.833 Ru/0.167 Ir. [b]Refined with an occupancy factor of 0.833. [c]Refined with an occupancy factor of 0.167. [d]Carbon atoms of this solvent benzene molecule were refined as an idealized hexagon (d(C–C) = 1.39 Å) with a common isotropic displacement parameter.

Table S-3. Selected Interatomic Distances (Å) for **2**

(a) involving 'inner-core' atoms of [IrRuH(CO)$_3$(μ–CO)(dppm)$_2$]

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ir	Ru	2.8091(3)	P(4)	C(6)	1.848(4)
Ir	P(1)	2.3029(10)	O(1)	C(1)	1.115(5)
Ir	P(3)	2.3117(10)	O(2)	C(2)	1.188(5)
Ir	C(1)	1.935(4)	O(3)	C(3)	1.148(6)
Ir	C(2)	2.063(4)	O(4)	C(4)	1.112(5)
Ru	P(2)	2.3361(10)	P(1)	C(11)	1.830(4)
Ru	P(4)	2.3360(10)	P(1)	C(21)	1.834(4)
Ru	C(2)	2.117(4)	P(2)	C(31)	1.828(4)
Ru	C(3)	1.925(5)	P(2)	C(41)	1.832(4)
Ru	C(4)	1.954(4)	P(3)	C(51)	1.845(4)
P(1)	C(5)	1.830(4)	P(3)	C(61)	1.823(4)
P(2)	C(5)	1.840(4)	P(4)	C(71)	1.835(4)
P(3)	C(6)	1.831(4)	P(4)	C(81)	1.839(4)

(b) involving dppm phenyl carbons

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C(11)	C(12)	1.401(6)	C(51)	C(52)	1.374(6)
C(11)	C(16)	1.381(6)	C(51)	C(56)	1.399(6)
C(12)	C(13)	1.375(7)	C(52)	C(53)	1.404(6)
C(13)	C(14)	1.374(8)	C(53)	C(54)	1.374(7)
C(14)	C(15)	1.368(8)	C(54)	C(55)	1.381(8)
C(15)	C(16)	1.390(6)	C(55)	C(56)	1.384(7)
C(21)	C(22)	1.378(6)	C(61)	C(62)	1.402(6)
C(21)	C(26)	1.393(6)	C(61)	C(66)	1.398(6)
C(22)	C(23)	1.396(7)	C(62)	C(63)	1.381(7)
C(23)	C(24)	1.365(8)	C(63)	C(64)	1.373(9)
C(24)	C(25)	1.346(8)	C(64)	C(65)	1.360(8)
C(25)	C(26)	1.393(6)	C(65)	C(66)	1.392(7)
C(31)	C(32)	1.390(5)	C(71)	C(72)	1.393(6)
C(31)	C(36)	1.391(6)	C(71)	C(76)	1.402(6)
C(32)	C(33)	1.399(6)	C(72)	C(73)	1.376(6)
C(33)	C(34)	1.388(6)	C(73)	C(74)	1.391(7)
C(34)	C(35)	1.383(7)	C(74)	C(75)	1.381(7)
C(35)	C(36)	1.373(6)	C(75)	C(76)	1.380(6)
C(41)	C(42)	1.384(6)	C(81)	C(82)	1.395(6)
C(41)	C(46)	1.385(6)	C(81)	C(86)	1.364(6)
C(42)	C(43)	1.385(7)	C(82)	C(83)	1.386(7)
C(43)	C(44)	1.375(7)	C(83)	C(84)	1.363(8)
C(44)	C(45)	1.363(7)	C(84)	C(85)	1.375(9)
C(45)	C(46)	1.396(7)	C(85)	C(86)	1.393(7)

(c) within the solvent benzene molecules

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C(11S)	C(12S)	1.368(9)	C(25S)	C(26S)	1.403(11)
C(11S)	C(16S)	1.355(11)	C(31S)	C(32S)	1.358(13)
C(12S)	C(13S)	1.355(9)	C(31S)	C(36S)	1.380(13)
C(13S)	C(14S)	1.345(11)	C(32S)	C(33S)	1.390(11)
C(14S)	C(15S)	1.404(11)	C(33S)	C(34S)	1.377(11)
C(15S)	C(16S)	1.402(11)	C(34S)	C(35S)	1.390(13)
C(21S)	C(22S)	1.345(11)	C(35S)	C(36S)	1.369(12)
C(21S)	C(26S)	1.373(11)	C(51S)	C(52S)	1.317(10)
C(22S)	C(23S)	1.342(10)	C(51S)	C(53S")	1.415(12)
C(23S)	C(24S)	1.341(10)	C(52S)	C(53S)	1.342(10)
C(24S)	C(25S)	1.355(10)			

Double-primed atoms are related to unprimed ones via the inversion center ($^{-1}/_2$, 0, $^1/_2$).

Table S-4. Selected Interatomic Angles (deg) for **2**

(a) involving 'inner-core' atoms of [IrRuH(CO)$_3$(μ–CO)(dppm)$_2$]

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ru	Ir	P(1)	94.62(3)	Ru	P(2)	C(5)	113.61(13)
Ru	Ir	P(3)	94.31(3)	Ir	P(3)	C(6)	110.15(13)
Ru	Ir	C(1)	99.36(12)	Ru	P(4)	C(6)	113.20(13)
Ru	Ir	C(2)	48.60(11)	Ir	C(1)	O(1)	174.4(4)
P(1)	Ir	P(3)	167.34(4)	Ir	C(2)	Ru	84.43(14)
P(1)	Ir	C(1)	90.54(11)	Ir	C(2)	O(2)	138.8(3)
P(1)	Ir	C(2)	91.81(10)	Ru	C(2)	O(2)	136.7(3)
P(3)	Ir	C(1)	96.84(11)	Ru	C(3)	O(3)	178.7(5)
P(3)	Ir	C(2)	87.39(10)	Ru	C(4)	O(4)	178.1(4)
C(1)	Ir	C(2)	147.96(16)	P(1)	C(5)	P(2)	111.3(2)
Ir	Ru	P(2)	90.87(3)	P(3)	C(6)	P(4)	112.80(19)
Ir	Ru	P(4)	91.78(3)	Ir	P(1)	C(11)	113.95(13)
Ir	Ru	C(2)	46.97(10)	Ir	P(1)	C(21)	120.53(14)
Ir	Ru	C(3)	151.65(15)	C(5)	P(1)	C(11)	102.85(19)
Ir	Ru	C(4)	96.50(12)	C(5)	P(1)	C(21)	103.91(18)
P(2)	Ru	P(4)	176.95(4)	C(11)	P(1)	C(21)	102.68(18)
P(2)	Ru	C(2)	90.76(10)	Ru	P(2)	C(31)	119.72(13)
P(2)	Ru	C(3)	89.75(14)	Ru	P(2)	C(41)	116.47(13)
P(2)	Ru	C(4)	89.65(12)	C(5)	P(2)	C(31)	103.52(18)
P(4)	Ru	C(2)	89.96(10)	C(5)	P(2)	C(41)	101.52(18)
P(4)	Ru	C(3)	87.20(14)	C(31)	P(2)	C(41)	99.41(18)
P(4)	Ru	C(4)	91.54(12)	Ir	P(3)	C(51)	117.07(14)
C(2)	Ru	C(3)	104.68(18)	Ir	P(3)	C(61)	117.51(14)
C(2)	Ru	C(4)	143.47(16)	C(6)	P(3)	C(51)	101.39(19)
C(3)	Ru	C(4)	111.8(2)	C(6)	P(3)	C(61)	105.78(19)
Ir'	Ru'	C(3')	144.8(7)	C(51)	P(3)	C(61)	103.21(19)
P(1)	Ru'	C(3')	84.7(9)	Ru	P(4)	C(71)	119.55(13)
P(3)	Ru'	C(3')	82.8(9)	Ru	P(4)	C(81)	115.37(13)
C(1)	Ru'	C(3')	115.9(7)	C(6)	P(4)	C(71)	102.90(18)
C(2)	Ru'	C(3')	96.2(7)	C(6)	P(4)	C(81)	102.94(18)
Ir	P(1)	C(5)	111.02(13)	C(71)	P(4)	C(81)	100.67(18)

(b) involving dppm phenyl carbons

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P(1)	C(11)	C(12)	117.6(3)	C(33)	C(34)	C(35)	120.1(4)
P(1)	C(11)	C(16)	124.3(3)	C(34)	C(35)	C(36)	120.0(4)
C(12)	C(11)	C(16)	118.0(4)	C(31)	C(36)	C(35)	121.1(4)
C(11)	C(12)	C(13)	120.4(5)	P(2)	C(41)	C(42)	117.8(3)
C(12)	C(13)	C(14)	121.0(5)	P(2)	C(41)	C(46)	124.3(3)
C(13)	C(14)	C(15)	119.3(5)	C(42)	C(41)	C(46)	117.8(4)
C(14)	C(15)	C(16)	120.5(5)	C(41)	C(42)	C(43)	120.9(5)
C(11)	C(16)	C(15)	120.8(5)	C(42)	C(43)	C(44)	120.7(5)
P(1)	C(21)	C(22)	121.5(3)	C(43)	C(44)	C(45)	119.1(4)
P(1)	C(21)	C(26)	119.5(3)	C(44)	C(45)	C(46)	120.6(5)
C(22)	C(21)	C(26)	118.9(4)	C(41)	C(46)	C(45)	120.8(5)
C(21)	C(22)	C(23)	119.7(5)	P(3)	C(51)	C(52)	121.3(3)
C(22)	C(23)	C(24)	120.6(5)	P(3)	C(51)	C(56)	119.4(3)
C(23)	C(24)	C(25)	120.1(5)	C(52)	C(51)	C(56)	119.4(4)
C(24)	C(25)	C(26)	120.8(5)	C(51)	C(52)	C(53)	120.4(4)
C(21)	C(26)	C(25)	119.8(5)	C(52)	C(53)	C(54)	119.7(5)
P(2)	C(31)	C(32)	120.4(3)	C(53)	C(54)	C(55)	120.2(4)
P(2)	C(31)	C(36)	120.5(3)	C(54)	C(55)	C(56)	120.2(5)
C(32)	C(31)	C(36)	119.0(4)	C(51)	C(56)	C(55)	120.0(5)
C(31)	C(32)	C(33)	120.0(4)	P(3)	C(61)	C(62)	120.1(4)
C(32)	C(33)	C(34)	119.7(4)	P(3)	C(61)	C(66)	122.8(4)

Table S-4. Selected Interatomic Angles for **2** (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C(62)	C(61)	C(66)	117.0(4)	C(73)	C(74)	C(75)	119.1(4)
C(61)	C(62)	C(63)	121.0(5)	C(74)	C(75)	C(76)	120.0(4)
C(62)	C(63)	C(64)	120.5(5)	C(71)	C(76)	C(75)	121.2(4)
C(63)	C(64)	C(65)	120.0(5)	P(4)	C(81)	C(82)	117.8(3)
C(64)	C(65)	C(66)	120.4(5)	P(4)	C(81)	C(86)	123.6(4)
C(61)	C(66)	C(65)	121.1(5)	C(82)	C(81)	C(86)	118.6(4)
P(4)	C(71)	C(72)	121.9(3)	C(81)	C(82)	C(83)	120.4(5)
P(4)	C(71)	C(76)	119.7(3)	C(82)	C(83)	C(84)	120.3(5)
C(72)	C(71)	C(76)	118.4(4)	C(83)	C(84)	C(85)	119.8(5)
C(71)	C(72)	C(73)	120.0(4)	C(84)	C(85)	C(86)	119.9(5)
C(72)	C(73)	C(74)	121.4(4)	C(81)	C(86)	C(85)	120.9(5)

(c) within the solvent benzene molecules

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C(12S)	C(11S)	C(16S)	121.1(7)	C(21S)	C(26S)	C(25S)	119.4(8)
C(11S)	C(12S)	C(13S)	120.3(8)	C(32S)	C(31S)	C(36S)	118.5(9)
C(12S)	C(13S)	C(14S)	120.7(7)	C(31S)	C(32S)	C(33S)	121.8(9)
C(13S)	C(14S)	C(15S)	120.3(7)	C(32S)	C(33S)	C(34S)	119.0(10)
C(14S)	C(15S)	C(16S)	118.4(8)	C(33S)	C(34S)	C(35S)	119.8(9)
C(11S)	C(16S)	C(15S)	119.2(7)	C(34S)	C(35S)	C(36S)	119.5(9)
C(22S)	C(21S)	C(26S)	118.7(8)	C(31S)	C(36S)	C(35S)	121.4(10)
C(21S)	C(22S)	C(23S)	122.3(8)	C(52S)	C(51S)	C(53S")	119.5(8)
C(22S)	C(23S)	C(24S)	119.9(8)	C(51S)	C(52S)	C(53S)	121.2(8)
C(23S)	C(24S)	C(25S)	121.0(7)	C(51S")	C(53S)	C(52S)	118.9(7)
C(24S)	C(25S)	C(26S)	118.8(7)				

Double-primed atoms are related to unprimed ones via the inversion center ($^{-1}/_{2}$, 0, $^{1}/_{2}$).

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir/Ru'	0.02273(9)	0.02165(9)	0.03221(10)	0.00208(6)	-0.00779(7)	-0.00953(6)
Ru/Ir'	0.02794(15)	0.02722(15)	0.02825(15)	-0.00013(11)	-0.00437(11)	-0.01314(12)
P(1)	0.0234(5)	0.0234(5)	0.0317(5)	-0.0005(4)	-0.0071(4)	-0.0092(4)
P(2)	0.0249(5)	0.0225(5)	0.0249(5)	0.0001(4)	-0.0067(4)	-0.0086(4)
P(3)	0.0264(5)	0.0211(5)	0.0326(5)	0.0013(4)	-0.0092(4)	-0.0083(4)
P(4)	0.0226(5)	0.0249(5)	0.0281(5)	0.0025(4)	-0.0061(4)	-0.0086(4)
O(1)	0.079(3)	0.053(2)	0.056(2)	0.0101(18)	-0.034(2)	-0.031(2)
O(2)	0.0423(17)	0.0361(16)	0.0276(15)	0.0037(12)	-0.0070(13)	-0.0127(14)
O(3)	0.041(2)	0.030(2)	0.084(3)	0.015(2)	-0.031(2)	-0.0054(18)
O(3')	0.088(19)	0.076(17)	0.065(16)	0.022(14)	-0.029(14)	-0.041(15)
O(4)	0.061(2)	0.073(3)	0.040(2)	0.0060(18)	-0.0136(17)	-0.021(2)
C(1)	0.034(2)	0.024(2)	0.036(2)	0.0047(17)	-0.0152(18)	-0.0143(17)
C(2)	0.026(2)	0.0237(19)	0.032(2)	0.0039(16)	-0.0074(16)	-0.0137(16)
C(3)	0.027(3)	0.028(3)	0.040(3)	0.005(2)	-0.009(2)	-0.012(2)
C(4)	0.026(2)	0.035(2)	0.030(2)	-0.0003(17)	-0.0025(17)	-0.0104(18)
C(5)	0.026(2)	0.028(2)	0.0276(19)	0.0003(16)	-0.0087(16)	-0.0091(17)
C(6)	0.028(2)	0.0256(19)	0.0269(19)	0.0015(16)	-0.0051(16)	-0.0124(17)
C(11)	0.0210(19)	0.032(2)	0.041(2)	0.0067(18)	-0.0059(17)	-0.0130(17)
C(12)	0.034(2)	0.031(2)	0.069(3)	-0.006(2)	-0.018(2)	-0.007(2)
C(13)	0.040(3)	0.033(3)	0.085(4)	0.005(3)	-0.019(3)	-0.005(2)
C(14)	0.031(3)	0.055(3)	0.074(4)	0.026(3)	-0.021(3)	-0.011(2)
C(15)	0.034(3)	0.067(4)	0.048(3)	0.010(3)	-0.017(2)	-0.012(2)
C(16)	0.029(2)	0.045(3)	0.042(2)	0.002(2)	-0.0099(19)	-0.009(2)
C(21)	0.028(2)	0.030(2)	0.031(2)	-0.0002(17)	-0.0037(17)	-0.0093(17)
C(22)	0.047(3)	0.077(4)	0.033(2)	-0.004(2)	-0.002(2)	-0.035(3)
C(23)	0.068(4)	0.124(6)	0.033(3)	0.003(3)	-0.007(3)	-0.047(4)
C(24)	0.057(3)	0.079(4)	0.046(3)	0.014(3)	-0.002(3)	-0.037(3)
C(25)	0.059(3)	0.063(3)	0.047(3)	0.009(3)	-0.003(2)	-0.039(3)
C(26)	0.050(3)	0.047(3)	0.042(3)	0.003(2)	-0.010(2)	-0.028(2)
C(31)	0.031(2)	0.026(2)	0.028(2)	0.0034(16)	-0.0092(17)	-0.0117(17)
C(32)	0.044(3)	0.028(2)	0.034(2)	0.0027(17)	-0.0136(19)	-0.0150(19)
C(33)	0.059(3)	0.041(3)	0.033(2)	0.0069(19)	-0.018(2)	-0.021(2)
C(34)	0.055(3)	0.033(2)	0.036(2)	0.0089(19)	-0.010(2)	-0.018(2)
C(35)	0.054(3)	0.044(3)	0.050(3)	0.018(2)	-0.017(2)	-0.032(2)
C(36)	0.055(3)	0.044(3)	0.037(2)	0.009(2)	-0.020(2)	-0.029(2)
C(41)	0.032(2)	0.027(2)	0.027(2)	0.0002(16)	-0.0044(17)	-0.0134(17)
C(42)	0.042(3)	0.046(3)	0.055(3)	-0.017(2)	-0.019(2)	-0.001(2)
C(43)	0.046(3)	0.040(3)	0.071(4)	-0.019(3)	-0.019(3)	0.004(2)
C(44)	0.057(3)	0.038(3)	0.039(3)	-0.012(2)	-0.005(2)	-0.017(2)
C(45)	0.070(4)	0.048(3)	0.040(3)	-0.009(2)	-0.024(3)	-0.016(3)
C(46)	0.048(3)	0.038(2)	0.038(2)	-0.004(2)	-0.018(2)	-0.005(2)
C(51)	0.038(2)	0.027(2)	0.039(2)	0.0068(18)	-0.0139(19)	-0.0130(18)
C(52)	0.040(3)	0.026(2)	0.059(3)	0.001(2)	-0.018(2)	-0.008(2)
C(53)	0.054(3)	0.031(2)	0.078(4)	0.008(2)	-0.034(3)	-0.006(2)
C(54)	0.067(4)	0.027(2)	0.076(4)	0.018(2)	-0.028(3)	-0.012(2)
C(55)	0.062(4)	0.034(3)	0.109(5)	0.022(3)	-0.041(4)	-0.025(3)
C(56)	0.052(3)	0.040(3)	0.087(4)	0.018(3)	-0.035(3)	-0.025(2)
C(61)	0.044(3)	0.020(2)	0.038(2)	-0.0020(17)	-0.016(2)	-0.0057(18)
C(62)	0.063(3)	0.036(3)	0.040(3)	0.001(2)	-0.009(2)	-0.021(2)
C(63)	0.096(5)	0.041(3)	0.038(3)	0.001(2)	-0.011(3)	-0.023(3)
C(64)	0.100(5)	0.042(3)	0.045(3)	-0.002(2)	-0.031(3)	-0.006(3)
C(65)	0.071(4)	0.049(3)	0.069(4)	-0.009(3)	-0.045(3)	-0.004(3)
C(66)	0.046(3)	0.040(3)	0.046(3)	-0.005(2)	-0.019(2)	-0.007(2)
C(71)	0.025(2)	0.026(2)	0.034(2)	0.0012(17)	-0.0090(17)	-0.0039(17)
C(72)	0.034(2)	0.041(2)	0.040(2)	0.011(2)	-0.0127(19)	-0.014(2)

Table S-5. Anisotropic Displacement Parameters for **2** (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(73)	0.042(3)	0.058(3)	0.040(3)	0.015(2)	-0.015(2)	-0.013(2)
C(74)	0.045(3)	0.059(3)	0.048(3)	0.004(2)	-0.025(2)	-0.014(2)
C(75)	0.040(3)	0.052(3)	0.046(3)	-0.003(2)	-0.018(2)	-0.019(2)
C(76)	0.036(2)	0.037(2)	0.040(2)	0.0043(19)	-0.011(2)	-0.014(2)
C(81)	0.027(2)	0.037(2)	0.031(2)	-0.0048(18)	-0.0034(17)	-0.0126(18)
C(82)	0.033(2)	0.048(3)	0.045(3)	-0.007(2)	-0.005(2)	-0.004(2)
C(83)	0.031(3)	0.063(3)	0.056(3)	-0.015(3)	-0.003(2)	-0.007(2)
C(84)	0.044(3)	0.074(4)	0.053(3)	-0.021(3)	0.019(3)	-0.027(3)
C(85)	0.064(4)	0.071(4)	0.048(3)	0.012(3)	0.015(3)	-0.020(3)
C(86)	0.046(3)	0.050(3)	0.044(3)	0.011(2)	0.002(2)	-0.011(2)
C(11S)	0.084(5)	0.087(5)	0.078(5)	0.032(4)	-0.033(4)	-0.038(4)
C(12S)	0.079(5)	0.078(5)	0.085(5)	0.019(4)	-0.030(4)	-0.033(4)
C(13S)	0.072(5)	0.086(5)	0.098(6)	0.024(4)	-0.027(4)	-0.042(4)
C(14S)	0.072(5)	0.109(6)	0.090(5)	0.009(5)	-0.022(4)	-0.044(5)
C(15S)	0.094(6)	0.081(5)	0.133(8)	-0.026(5)	-0.071(6)	0.000(5)
C(16S)	0.107(6)	0.075(5)	0.102(6)	0.033(5)	-0.064(5)	-0.039(5)
C(21S)	0.101(6)	0.052(4)	0.125(7)	-0.003(4)	-0.059(6)	-0.011(4)
C(22S)	0.061(4)	0.091(6)	0.097(6)	-0.031(5)	-0.028(4)	-0.019(4)
C(23S)	0.074(5)	0.088(5)	0.075(4)	-0.007(4)	-0.037(4)	-0.028(4)
C(24S)	0.071(4)	0.057(4)	0.105(6)	-0.001(4)	-0.053(4)	-0.012(3)
C(25S)	0.056(4)	0.074(5)	0.111(6)	-0.034(4)	-0.011(4)	-0.016(4)
C(26S)	0.121(7)	0.091(6)	0.089(5)	0.008(5)	-0.033(5)	-0.060(6)
C(31S)	0.055(5)	0.090(6)	0.200(12)	0.023(7)	-0.027(6)	-0.015(5)
C(32S)	0.100(7)	0.097(6)	0.140(8)	0.032(6)	-0.046(6)	-0.044(6)
C(33S)	0.140(8)	0.061(5)	0.115(7)	0.013(4)	-0.041(6)	-0.045(5)
C(34S)	0.169(9)	0.072(5)	0.081(5)	0.003(4)	-0.030(6)	-0.038(6)
C(35S)	0.154(9)	0.099(7)	0.099(7)	0.022(6)	-0.050(7)	-0.037(7)
C(36S)	0.088(6)	0.092(6)	0.137(9)	0.001(6)	-0.017(6)	-0.025(5)
C(51S)	0.105(6)	0.056(5)	0.204(11)	-0.023(5)	-0.087(7)	-0.002(4)
C(52S)	0.097(6)	0.068(5)	0.148(8)	-0.002(5)	-0.074(6)	-0.020(4)
C(53S)	0.160(9)	0.056(4)	0.132(7)	0.010(4)	-0.095(7)	-0.023(5)

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 **2**

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(5A)	0.1450	0.4585	0.2743	0.032
H(5B)	0.0848	0.4081	0.3465	0.032
H(6A)	-0.2151	0.1817	0.3500	0.032
H(6B)	-0.2582	0.1623	0.2804	0.032
H(12)	0.2953	0.1437	0.1804	0.054
H(13)	0.4311	0.0607	0.2191	0.065
H(14)	0.4705	0.1166	0.3236	0.063
H(15)	0.3796	0.2609	0.3842	0.059
H(16)	0.2462	0.3479	0.3435	0.047
H(22)	0.1544	0.2901	0.0598	0.062
H(23)	0.2345	0.3446	-0.0624	0.088
H(24)	0.3540	0.4256	-0.0711	0.073
H(25)	0.3861	0.4624	0.0419	0.067
H(26)	0.3021	0.4155	0.1665	0.054
H(32)	-0.0717	0.5055	0.1323	0.041
H(33)	-0.0232	0.5894	0.0215	0.050
H(34)	0.0803	0.6860	0.0214	0.050
H(35)	0.1380	0.6965	0.1297	0.055
H(36)	0.0926	0.6120	0.2377	0.050
H(42)	-0.2002	0.6428	0.3340	0.059
H(43)	-0.2543	0.7671	0.4270	0.067
H(44)	-0.1645	0.7755	0.5150	0.056
H(45)	-0.0186	0.6597	0.5079	0.061
H(46)	0.0347	0.5328	0.4166	0.050
H(52)	0.0866	0.0385	0.2753	0.050
H(53)	0.1218	-0.1070	0.3183	0.063
H(54)	0.0122	-0.1971	0.3202	0.067
H(55)	-0.1301	-0.1450	0.2768	0.076
H(56)	-0.1673	0.0000	0.2361	0.065
H(62)	0.0589	0.1420	0.0605	0.057
H(63)	0.0513	0.1145	-0.0662	0.073
H(64)	-0.1015	0.0981	-0.0800	0.076
H(65)	-0.2452	0.1026	0.0330	0.072
H(66)	-0.2380	0.1234	0.1615	0.053
H(72)	-0.2285	0.3908	0.1352	0.045
H(73)	-0.2934	0.3860	0.0312	0.056
H(74)	-0.4281	0.3188	0.0435	0.058
H(75)	-0.4976	0.2550	0.1625	0.053
H(76)	-0.4301	0.2556	0.2659	0.045
H(82)	-0.4541	0.4581	0.3378	0.055
H(83)	-0.6100	0.4996	0.4476	0.065
H(84)	-0.6329	0.4169	0.5584	0.076
H(85)	-0.5023	0.2889	0.5587	0.084
H(86)	-0.3484	0.2439	0.4469	0.062
H(11S)	-0.0821	0.0770	0.4502	0.094
H(12S)	-0.1012	-0.0583	0.4996	0.093
H(13S)	-0.2342	-0.0611	0.6174	0.098
H(14S)	-0.3584	0.0689	0.6808	0.106
H(15S)	-0.3411	0.2091	0.6332	0.119
H(16S)	-0.1980	0.2111	0.5158	0.102
H(21S)	0.2475	-0.2569	0.2293	0.108
H(22S)	0.1795	-0.3151	0.3483	0.100
H(23S)	0.2512	-0.4584	0.3707	0.090
H(24S)	0.4006	-0.5455	0.2766	0.088
H(25S)	0.4780	-0.4912	0.1564	0.102

Table S-6. Derived Parameters for Hydrogen Atoms of **2** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(26S)	0.4013	-0.3432	0.1321	0.114
H(31S)	0.3793	-0.0190	-0.2116	0.145
H(32S)	0.2481	0.0612	-0.0984	0.129
H(33S)	0.1749	0.2156	-0.0958	0.123
H(34S)	0.2417	0.2913	-0.2074	0.131
H(35S)	0.3822	0.2116	-0.3196	0.138
H(36S)	0.4426	0.0569	-0.3236	0.134
H(41S)	-0.2798	-0.0202	-0.0555	0.220
H(42S)	-0.2667	0.0394	-0.1795	0.220
H(43S)	-0.4010	0.1602	-0.1894	0.220
H(44S)	-0.5484	0.2214	-0.0753	0.220
H(45S)	-0.5614	0.1619	0.0487	0.220
H(46S)	-0.4271	0.0411	0.0586	0.220
H(51S)	-0.3329	-0.0785	0.4918	0.140
H(52S)	-0.3711	0.0722	0.4841	0.115
H(53S)	-0.5294	0.1497	0.4757	0.127

Table S-7. Crystallographic Experimental Details for **5**

A. Crystal Data	
formula	$C_{56}H_{48}BCl_2F_4IrO_4P_4Ru$
formula weight	1359.80
crystal dimensions (mm)	0.26 × 0.15 × 0.04
crystal system	monoclinic
space group	$P2_1/n$ (a nonstandard setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	12.5470 (7)
b (Å)	27.1409 (13)
c (Å)	15.9168 (9)
β (deg)	96.4809 (10)
V (Å^3)	5385.6 (5)
Z	4
ρ_{calcd} (g cm^{-3})	1.677
μ (mm^{-1})	3.027
B. Data Collection and Refinement Conditions	
diffractometer	Bruker P4/RA/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ϕ rotations (0.3°) / ω scans (0.3°) (30 s exposures)
data collection 2θ limit (deg)	52.82
total data collected	26607 ($-15 \le h \le 15$, $-12 \le k \le 33$, $-19 \le l \le 19$)
independent reflections	11017
number of observations (*NO*)	6835 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	*SADABS*
range of transmission factors	0.8943–0.5913
data/restraints/parameters	11017 [$F_o^2 \ge -3\sigma(F_o^2)$] / 17[e] / 641
goodness-of-fit (*S*)[f]	0.997 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0549
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1617
largest difference peak and hole	1.469 and –1.529 e Å^{-3}

[a]Obtained from least-squares refinement of 6519 centered reflections.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

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

(continued)

Table S–7. Crystallographic Experimental Details for **5** (continued)

[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]The distances of C(5') to Ir' (2.05 Å) and Ru' (2.31 Å) were given fixed values based on the corresponding Ir–C(5) and Ru–C(5) distances. Distances within the BF_4^- ion (F–B = 1.35 A; F···F = 2.20 Å) and the disordered solvent CH_2Cl_2 molecule (Cl–C = 1.80 Å; Cl···Cl = 2.95 Å) were given fixed idealized values.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0812P)^2]^{-1}$ 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 Equivalent Isotropic Displacement Parameters for **5**

(a) 'inner-core' atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ir/Ru'[a]	-0.15920(3)	0.004230(11)	-0.29634(2)	0.03223(12)*
Ru/Ir'[b]	-0.28565(4)	0.007956(17)	-0.15743(4)	0.03507(15)*
P(1)	-0.07421(16)	-0.06966(7)	-0.24976(13)	0.0283(5)*
P(2)	-0.22259(17)	-0.07079(7)	-0.10999(13)	0.0314(5)*
P(3)	-0.20039(17)	0.08610(7)	-0.33571(13)	0.0305(5)*
P(4)	-0.34825(18)	0.08766(7)	-0.19656(14)	0.0347(5)*
O(1)	-0.1464(6)	-0.0234(2)	-0.4778(4)	0.0600(18)*
O(2)	-0.3815(5)	-0.0370(2)	-0.3251(4)	0.0475(15)*
O(3)	-0.5039(5)	-0.0125(2)	-0.1001(4)	0.0545(17)*
O(4)[c]	-0.1708(9)	0.0492(3)	0.0133(6)	0.079(3)*
O(4')[d]	0.092(2)	0.0417(11)	-0.296(2)	0.092(11)*
C(1)	-0.1566(8)	-0.0138(3)	-0.4093(6)	0.046(2)*
C(2)	-0.3110(6)	-0.0173(3)	-0.2809(5)	0.0329(19)*
C(3)	-0.4240(7)	-0.0058(3)	-0.1227(6)	0.040(2)*
C(4)[c]	-0.2155(12)	0.0344(4)	-0.0490(8)	0.060(4)*
C(4')[d]	0.004(4)	0.0317(15)	-0.283(6)	0.16(4)*
C(5)[c]	-0.1129(10)	0.0302(6)	-0.1772(8)	0.042(3)*
C(5')[d,e]	-0.132(2)	0.034(2)	-0.1595(15)	0.050
C(6)	-0.0871(6)	-0.0829(3)	-0.1384(5)	0.0327(18)*
C(7)	-0.2511(7)	0.1228(3)	-0.2508(5)	0.038(2)*

(b) dppm phenyl carbons

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(11)	0.0701(6)	-0.0704(3)	-0.2568(5)	0.0351(19)*
C(12)	0.1454(8)	-0.0872(4)	-0.1927(6)	0.054(3)*
C(13)	0.2553(8)	-0.0876(4)	-0.2034(7)	0.058(3)*
C(14)	0.2877(8)	-0.0732(3)	-0.2781(7)	0.055(3)*
C(15)	0.2143(10)	-0.0574(5)	-0.3428(7)	0.086(4)*
C(16)	0.1066(8)	-0.0565(5)	-0.3315(6)	0.080(4)*
C(21)	-0.1205(7)	-0.1271(3)	-0.3020(5)	0.0335(19)*
C(22)	-0.2129(7)	-0.1287(3)	-0.3583(5)	0.037(2)*
C(23)	-0.2496(7)	-0.1732(3)	-0.3952(6)	0.046(2)*
C(24)	-0.1907(8)	-0.2154(3)	-0.3781(6)	0.052(3)*
C(25)	-0.0949(9)	-0.2141(3)	-0.3249(7)	0.062(3)*
C(26)	-0.0595(8)	-0.1697(3)	-0.2857(6)	0.054(3)*
C(31)	-0.2992(7)	-0.1239(3)	-0.1509(6)	0.040(2)*
C(32)	-0.4026(7)	-0.1199(3)	-0.1936(5)	0.039(2)*
C(33)	-0.4585(9)	-0.1609(3)	-0.2289(6)	0.056(3)*
C(34)	-0.4108(10)	-0.2063(3)	-0.2197(8)	0.077(4)*
C(35)	-0.3077(10)	-0.2120(3)	-0.1765(9)	0.087(4)*
C(36)	-0.2531(8)	-0.1714(3)	-0.1415(8)	0.071(3)*
C(41)	-0.2084(7)	-0.0797(3)	0.0039(5)	0.044(2)*
C(42)	-0.1324(12)	-0.1117(5)	0.0440(8)	0.115(6)*
C(43)	-0.1281(16)	-0.1179(7)	0.1316(9)	0.180(10)*
C(44)	-0.1880(13)	-0.0928(7)	0.1805(8)	0.120(6)*
C(45)	-0.2629(10)	-0.0618(5)	0.1404(7)	0.085(4)*
C(46)	-0.2721(9)	-0.0550(4)	0.0545(7)	0.068(3)*
C(51)	-0.0903(7)	0.1221(3)	-0.3667(5)	0.036(2)*
C(52)	-0.0385(7)	0.1596(3)	-0.3174(6)	0.048(2)*
C(53)	0.0465(9)	0.1849(4)	-0.3464(7)	0.067(3)*
C(54)	0.0798(8)	0.1752(3)	-0.4213(7)	0.051(3)*
C(55)	0.0324(10)	0.1381(5)	-0.4680(8)	0.092(4)*
C(56)	-0.0522(9)	0.1118(4)	-0.4416(7)	0.085(4)*

Table S-8. Atomic Coordinates and Displacement Parameters for **5** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(61)	-0.3038(6)	0.0950(3)	-0.4239(5)	0.0312(18)*
C(62)	-0.3622(7)	0.0561(3)	-0.4594(5)	0.039(2)*
C(63)	-0.4439(7)	0.0641(3)	-0.5258(5)	0.044(2)*
C(64)	-0.4678(8)	0.1105(4)	-0.5556(6)	0.053(3)*
C(65)	-0.4073(8)	0.1496(3)	-0.5196(6)	0.058(3)*
C(66)	-0.3257(8)	0.1426(3)	-0.4565(6)	0.054(3)*
C(71)	-0.4702(7)	0.0943(3)	-0.2672(5)	0.038(2)*
C(72)	-0.5348(8)	0.0535(3)	-0.2952(5)	0.048(2)*
C(73)	-0.6273(8)	0.0595(4)	-0.3510(6)	0.065(3)*
C(74)	-0.6596(9)	0.1050(4)	-0.3810(7)	0.069(3)*
C(75)	-0.5958(10)	0.1456(4)	-0.3528(8)	0.082(4)*
C(76)	-0.5036(9)	0.1402(3)	-0.2974(8)	0.069(3)*
C(81)	-0.3728(8)	0.1265(3)	-0.1070(6)	0.045(2)*
C(82)	-0.2891(8)	0.1492(3)	-0.0567(6)	0.051(2)*
C(83)	-0.3093(11)	0.1747(3)	0.0145(6)	0.066(3)*
C(84)	-0.4091(13)	0.1779(4)	0.0383(7)	0.080(4)*
C(85)	-0.4914(11)	0.1557(5)	-0.0103(7)	0.083(4)*
C(86)	-0.4750(10)	0.1297(4)	-0.0831(7)	0.068(3)*
(c) tetrafluoroborate ion atoms				
Atom	*x*	*y*	*z*	U_{eq}, Å^2
F(1)	-0.0408(5)	0.17827(18)	0.0493(4)	0.093(2)
F(2)	-0.0940(5)	0.25360(19)	0.0151(4)	0.106(2)
F(3)	0.0713(4)	0.2303(3)	0.0003(5)	0.160(4)
F(4)	-0.0638(7)	0.2009(3)	-0.0848(3)	0.182(4)
B	-0.0319(4)	0.21580(19)	-0.0052(3)	0.163(10)
(d) solvent dichloromethane atoms				
Atom	*x*	*y*	*z*	U_{eq}, Å^2
Cl(1S)[f]	-0.1537(7)	0.2359(3)	0.4436(4)	0.247(2)
Cl(2S)[f]	-0.2342(6)	0.2310(3)	0.2627(4)	0.247(2)
C(1SA)[f,g]	-0.244(3)	0.2629(10)	0.3605(7)	0.247(2)
C(1SB)[f,h]	-0.239(5)	0.2027(17)	0.3644(9)	0.247(2)

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 as 75% Ir/25% Ru. [b]Refined as 75% Ir/25% Ru. [c]Refined with an occupancy factor of 0.75. [d]Refined with an occupancy factor of 0.25. [e]Refined with a fixed isotropic displacement parameter. [f]Atoms of the solvent molecule were refined with a common isotropic displacement parameter. [g]Refined with an occupancy factor of 0.65. [g]Refined with an occupancy factor of 0.35.

Table S–9. Selected Interatomic Distances for **5** (Å)

(a) involving 'inner-core' atoms

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ir	Ru	2.8650(7)	Ru	C(5)	2.305(12)
Ir	P(1)	2.3516(19)	Ru'	C(4')	2.17(5)
Ir	P(3)	2.3503(19)	Ru'	C(5')	2.31†
Ir	C(1)	1.868(9)	O(1)	C(1)	1.141(10)
Ir	C(2)	2.033(8)	O(2)	C(2)	1.194(9)
Ir	C(5)	2.045(11)	O(3)	C(3)	1.119(10)
Ir'	C(5')	2.05†	O(4)	C(4)	1.155(13)
Ru	P(2)	2.3726(19)	O(4')	C(4')	1.17(5)
Ru	P(4)	2.361(2)	P(1)	C(6)	1.834(8)
Ru	C(2)	2.072(8)	P(2)	C(6)	1.837(8)
Ru	C(3)	1.916(10)	P(3)	C(7)	1.848(8)
Ru	C(4)	1.981(12)	P(4)	C(7)	1.838(8)

†Distance fixed during refinement.

(b) involving dppm phenyl carbons

Atom1	Atom2	Distance	Atom1	Atom2	Distance
P(1)	C(11)	1.826(8)	C(42)	C(43)	1.400(17)
P(1)	C(21)	1.831(8)	C(43)	C(44)	1.329(18)
P(2)	C(31)	1.813(9)	C(44)	C(45)	1.365(16)
P(2)	C(41)	1.818(9)	C(45)	C(46)	1.373(14)
P(3)	C(51)	1.806(8)	C(51)	C(52)	1.399(11)
P(3)	C(61)	1.818(8)	C(51)	C(56)	1.363(12)
P(4)	C(71)	1.802(9)	C(52)	C(53)	1.391(12)
P(4)	C(81)	1.828(8)	C(53)	C(54)	1.333(13)
C(11)	C(12)	1.387(12)	C(54)	C(55)	1.349(14)
C(11)	C(16)	1.375(12)	C(55)	C(56)	1.382(14)
C(12)	C(13)	1.407(13)	C(61)	C(62)	1.368(10)
C(13)	C(14)	1.358(13)	C(61)	C(66)	1.409(10)
C(14)	C(15)	1.370(14)	C(62)	C(63)	1.405(11)
C(15)	C(16)	1.384(14)	C(63)	C(64)	1.367(12)
C(21)	C(22)	1.383(11)	C(64)	C(65)	1.391(13)
C(21)	C(26)	1.395(11)	C(65)	C(66)	1.365(13)
C(22)	C(23)	1.398(10)	C(71)	C(72)	1.414(12)
C(23)	C(24)	1.373(12)	C(71)	C(76)	1.383(11)
C(24)	C(25)	1.391(13)	C(72)	C(73)	1.389(13)
C(25)	C(26)	1.405(12)	C(73)	C(74)	1.368(14)
C(31)	C(32)	1.399(12)	C(74)	C(75)	1.406(15)
C(31)	C(36)	1.414(12)	C(75)	C(76)	1.381(15)
C(32)	C(33)	1.400(11)	C(81)	C(82)	1.390(13)
C(33)	C(34)	1.370(13)	C(81)	C(86)	1.381(13)
C(34)	C(35)	1.403(16)	C(82)	C(83)	1.377(13)
C(35)	C(36)	1.380(14)	C(83)	C(84)	1.352(16)
C(41)	C(42)	1.389(14)	C(84)	C(85)	1.359(16)
C(41)	C(46)	1.372(12)	C(85)	C(86)	1.392(13)

Table S–10. Selected Interatomic Angles for **5** (deg)

(a) involving 'inner-core' atoms

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ru	Ir	P(1)	93.31(5)	P(4)	Ru	C(5)	90.8(5)
Ru	Ir	P(3)	92.76(5)	C(2)	Ru	C(3)	99.3(3)
Ru	Ir	C(1)	145.5(3)	C(2)	Ru	C(4)	162.1(5)
Ru	Ir	C(2)	46.3(2)	C(2)	Ru	C(5)	90.2(3)
Ru	Ir	C(5)	52.9(3)	C(3)	Ru	C(4)	98.5(5)
P(1)	Ir	P(3)	165.59(7)	C(3)	Ru	C(5)	170.5(4)
P(1)	Ir	C(1)	91.3(2)	C(4)	Ru	C(5)	72.1(5)
P(1)	Ir	C(2)	96.5(2)	Ir'	Ru'	C(4')	121(2)
P(1)	Ir	C(5)	86.0(5)	Ir'	Ru'	C(5')	45.11(13)
P(3)	Ir	C(1)	91.1(2)	P(1)	Ru'	C(4')	82.7(11)
P(3)	Ir	C(2)	97.1(2)	P(1)	Ru'	C(5')	89.2(18)
P(3)	Ir	C(5)	87.3(5)	P(3)	Ru'	C(4')	83.0(11)
C(1)	Ir	C(2)	99.2(4)	P(3)	Ru'	C(5')	85.9(18)
C(1)	Ir	C(5)	161.7(5)	C(1)	Ru'	C(4')	94(2)
C(2)	Ir	C(5)	99.1(4)	C(1)	Ru'	C(5')	169.3(4)
Ru'	Ir'	C(5')	52.96(15)	C(2)	Ru'	C(4')	167(2)
P(2)	Ir'	C(5')	92(2)	C(2)	Ru'	C(5')	91.4(3)
P(4)	Ir'	C(5')	88(2)	C(4')	Ru'	C(5')	76(2)
C(2)	Ir'	C(5')	98.1(3)	C(4')	Ru'	C(5')	76(2)
C(3)	Ir'	C(5')	162.3(4)	Ir	P(1)	C(6)	112.6(2)
Ir	Ru	P(2)	91.14(5)	Ru	P(2)	C(6)	111.5(2)
Ir	Ru	P(4)	91.46(6)	Ir	P(3)	C(7)	113.4(3)
Ir	Ru	C(2)	45.2(2)	Ru	P(4)	C(7)	112.4(3)
Ir	Ru	C(3)	144.5(3)	Ir	C(1)	O(1)	174.3(9)
Ir	Ru	C(4)	117.1(4)	Ir	C(2)	Ru	88.5(3)
Ir	Ru	C(5)	45.0(3)	Ir	C(2)	O(2)	134.4(7)
P(2)	Ru	P(4)	176.76(8)	Ru	C(2)	O(2)	137.1(7)
P(2)	Ru	C(2)	90.8(2)	Ru	C(3)	O(3)	177.2(8)
P(2)	Ru	C(3)	90.7(2)	Ru	C(4)	O(4)	177.3(14)
P(2)	Ru	C(4)	87.1(3)	Ru'	C(4')	O(4')	163(7)
P(2)	Ru	C(5)	89.7(5)	Ir	C(5)	Ru	82.1(4)
P(4)	Ru	C(2)	92.4(2)	Ir'	C(5')	Ru'	81.93(17)
P(4)	Ru	C(3)	88.3(2)	P(1)	C(6)	P(2)	112.8(4)
P(4)	Ru	C(4)	90.0(3)	P(3)	C(7)	P(4)	111.4(4)

(b) involving dppm phenyl carbons

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ir	P(1)	C(11)	114.1(3)	C(7)	P(4)	C(81)	104.2(4)
Ir	P(1)	C(21)	118.3(3)	C(71)	P(4)	C(81)	102.9(4)
C(6)	P(1)	C(11)	104.7(4)	P(1)	C(11)	C(12)	123.8(7)
C(6)	P(1)	C(21)	102.4(4)	P(1)	C(11)	C(16)	118.7(7)
C(11)	P(1)	C(21)	103.2(4)	C(12)	C(11)	C(16)	117.4(8)
Ru	P(2)	C(31)	117.3(3)	C(11)	C(12)	C(13)	120.7(9)
Ru	P(2)	C(41)	115.4(3)	C(12)	C(13)	C(14)	119.8(9)
C(6)	P(2)	C(31)	103.8(4)	C(13)	C(14)	C(15)	120.5(10)
C(6)	P(2)	C(41)	103.4(4)	C(14)	C(15)	C(16)	119.4(11)
C(31)	P(2)	C(41)	103.9(4)	C(11)	C(16)	C(15)	122.2(10)
Ir	P(3)	C(51)	115.6(3)	P(1)	C(21)	C(22)	121.4(6)
Ir	P(3)	C(61)	116.6(2)	P(1)	C(21)	C(26)	118.8(7)
C(7)	P(3)	C(51)	104.2(4)	C(22)	C(21)	C(26)	119.8(8)
C(7)	P(3)	C(61)	102.7(4)	C(21)	C(22)	C(23)	120.8(8)
C(51)	P(3)	C(61)	102.7(4)	C(22)	C(23)	C(24)	119.5(9)
Ru	P(4)	C(71)	119.3(3)	C(23)	C(24)	C(25)	120.5(8)
Ru	P(4)	C(81)	113.8(3)	C(24)	C(25)	C(26)	120.1(8)
C(7)	P(4)	C(71)	102.5(4)	C(21)	C(26)	C(25)	119.2(9)

Table S–10. Selected Interatomic Angles for **5** (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P(2)	C(31)	C(32)	122.4(6)	P(3)	C(61)	C(62)	121.2(6)
P(2)	C(31)	C(36)	119.5(7)	P(3)	C(61)	C(66)	119.9(7)
C(32)	C(31)	C(36)	118.0(8)	C(62)	C(61)	C(66)	118.9(8)
C(31)	C(32)	C(33)	121.8(8)	C(61)	C(62)	C(63)	120.2(8)
C(32)	C(33)	C(34)	118.7(10)	C(62)	C(63)	C(64)	121.0(9)
C(33)	C(34)	C(35)	121.2(9)	C(63)	C(64)	C(65)	118.2(9)
C(34)	C(35)	C(36)	119.9(10)	C(64)	C(65)	C(66)	121.8(8)
C(31)	C(36)	C(35)	120.3(10)	C(61)	C(66)	C(65)	119.8(9)
P(2)	C(41)	C(42)	121.7(8)	P(4)	C(71)	C(72)	122.3(6)
P(2)	C(41)	C(46)	121.4(7)	P(4)	C(71)	C(76)	120.6(8)
C(42)	C(41)	C(46)	116.8(9)	C(72)	C(71)	C(76)	117.1(9)
C(41)	C(42)	C(43)	118.7(12)	C(71)	C(72)	C(73)	121.1(9)
C(42)	C(43)	C(44)	124.1(14)	C(72)	C(73)	C(74)	121.5(11)
C(43)	C(44)	C(45)	116.6(13)	C(73)	C(74)	C(75)	117.4(10)
C(44)	C(45)	C(46)	121.7(11)	C(74)	C(75)	C(76)	121.7(10)
C(41)	C(46)	C(45)	121.9(10)	C(71)	C(76)	C(75)	121.2(10)
P(3)	C(51)	C(52)	124.2(7)	P(4)	C(81)	C(82)	121.5(7)
P(3)	C(51)	C(56)	118.8(7)	P(4)	C(81)	C(86)	119.6(8)
C(52)	C(51)	C(56)	117.0(8)	C(82)	C(81)	C(86)	118.7(9)
C(51)	C(52)	C(53)	119.9(9)	C(81)	C(82)	C(83)	119.9(10)
C(52)	C(53)	C(54)	121.9(9)	C(82)	C(83)	C(84)	121.7(11)
C(53)	C(54)	C(55)	118.6(10)	C(83)	C(84)	C(85)	118.7(11)
C(54)	C(55)	C(56)	121.5(11)	C(84)	C(85)	C(86)	121.7(12)
C(51)	C(56)	C(55)	121.1(10)	C(81)	C(86)	C(85)	119.3(11)

Table S–11. Anisotropic Displacement Parameters for **5** (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir/Ru'	0.0431(2)	0.02697(17)	0.0263(2)	-0.00086(15)	0.00248(15)	0.00411(16)
Ru/Ir'	0.0340(3)	0.0300(3)	0.0415(3)	0.0038(2)	0.0056(2)	0.0037(2)
P(1)	0.0291(12)	0.0301(9)	0.0257(11)	-0.0001(8)	0.0031(9)	0.0031(8)
P(2)	0.0338(12)	0.0344(10)	0.0267(12)	0.0043(9)	0.0061(9)	0.0045(9)
P(3)	0.0371(13)	0.0268(9)	0.0286(12)	-0.0007(8)	0.0073(10)	0.0013(8)
P(4)	0.0428(14)	0.0286(9)	0.0338(13)	-0.0025(9)	0.0097(10)	0.0035(9)
O(1)	0.084(5)	0.056(4)	0.040(4)	0.003(3)	0.012(4)	0.023(4)
O(2)	0.041(4)	0.047(3)	0.053(4)	-0.001(3)	-0.002(3)	-0.001(3)
O(3)	0.039(4)	0.066(4)	0.061(5)	0.009(3)	0.022(3)	0.010(3)
O(4)	0.102(9)	0.074(6)	0.055(7)	-0.008(5)	-0.019(6)	-0.006(6)
O(4')	0.036(18)	0.07(2)	0.17(4)	0.01(2)	0.01(2)	0.014(16)
C(1)	0.078(7)	0.028(4)	0.032(5)	-0.007(3)	0.005(5)	0.017(4)
C(2)	0.031(5)	0.028(3)	0.038(5)	0.002(3)	-0.005(4)	0.003(3)
C(3)	0.040(5)	0.041(4)	0.037(5)	0.003(4)	0.002(4)	0.012(4)
C(4)	0.099(12)	0.039(6)	0.036(8)	-0.001(6)	-0.023(8)	-0.009(7)
C(4')	0.03(3)	0.04(2)	0.41(12)	0.05(4)	-0.01(5)	0.00(2)
C(5)	0.051(8)	0.044(6)	0.030(7)	-0.013(6)	0.009(6)	0.013(6)
C(6)	0.037(5)	0.035(4)	0.026(5)	0.001(3)	0.005(4)	0.004(3)
C(7)	0.036(5)	0.038(4)	0.040(5)	-0.008(4)	0.009(4)	-0.004(4)
C(11)	0.028(5)	0.043(4)	0.035(5)	0.000(4)	0.005(4)	-0.005(4)
C(12)	0.052(7)	0.064(6)	0.048(6)	0.010(5)	0.015(5)	0.009(5)
C(13)	0.039(6)	0.074(6)	0.059(7)	0.008(6)	-0.002(5)	0.008(5)
C(14)	0.032(6)	0.066(6)	0.071(8)	0.005(6)	0.018(5)	0.003(5)
C(15)	0.060(8)	0.149(12)	0.051(7)	0.008(8)	0.015(6)	0.004(8)
C(16)	0.031(6)	0.172(13)	0.034(6)	0.007(7)	-0.006(5)	-0.007(7)
C(21)	0.038(5)	0.032(4)	0.032(5)	0.004(3)	0.010(4)	0.002(3)
C(22)	0.037(5)	0.033(4)	0.042(5)	-0.004(4)	0.008(4)	-0.007(4)
C(23)	0.039(6)	0.046(5)	0.053(6)	-0.015(4)	0.007(5)	-0.009(4)
C(24)	0.068(7)	0.035(4)	0.056(7)	-0.011(4)	0.017(6)	-0.011(4)
C(25)	0.079(8)	0.030(4)	0.076(8)	0.002(5)	0.006(6)	0.016(5)
C(26)	0.073(7)	0.035(4)	0.054(7)	-0.001(4)	0.001(5)	0.007(4)
C(31)	0.036(5)	0.039(4)	0.047(6)	0.014(4)	0.010(4)	0.001(4)
C(32)	0.048(6)	0.041(4)	0.029(5)	0.004(4)	0.012(4)	-0.010(4)
C(33)	0.064(7)	0.049(5)	0.054(7)	0.005(5)	0.011(5)	-0.014(5)
C(34)	0.067(8)	0.043(5)	0.122(11)	-0.015(6)	0.013(8)	-0.023(5)
C(35)	0.079(9)	0.029(5)	0.157(14)	0.000(6)	0.029(9)	-0.006(5)
C(36)	0.045(7)	0.045(5)	0.125(11)	0.002(6)	0.024(7)	-0.001(5)
C(41)	0.046(6)	0.053(5)	0.036(5)	0.013(4)	0.013(4)	0.006(4)
C(42)	0.150(14)	0.139(12)	0.065(9)	0.050(9)	0.053(9)	0.086(11)
C(43)	0.24(2)	0.25(2)	0.055(10)	0.081(12)	0.039(12)	0.157(19)
C(44)	0.127(14)	0.194(17)	0.044(8)	0.024(9)	0.037(8)	0.075(12)
C(45)	0.072(9)	0.146(12)	0.041(7)	0.002(7)	0.022(6)	0.027(8)
C(46)	0.063(7)	0.095(8)	0.046(7)	0.008(6)	0.006(5)	0.036(6)
C(51)	0.040(5)	0.032(4)	0.039(5)	0.004(3)	0.012(4)	0.002(3)
C(52)	0.051(6)	0.049(5)	0.046(6)	-0.004(4)	0.013(5)	-0.015(4)
C(53)	0.067(8)	0.060(6)	0.074(8)	-0.016(6)	0.008(6)	-0.024(5)
C(54)	0.051(6)	0.042(4)	0.064(7)	-0.004(5)	0.020(5)	0.002(4)
C(55)	0.092(10)	0.121(10)	0.073(9)	-0.031(8)	0.056(7)	-0.046(8)
C(56)	0.084(9)	0.108(9)	0.070(8)	-0.040(7)	0.039(7)	-0.059(7)
C(61)	0.038(5)	0.036(4)	0.022(4)	0.003(3)	0.012(4)	0.009(3)
C(62)	0.042(5)	0.040(4)	0.034(5)	0.002(4)	0.004(4)	-0.001(4)
C(63)	0.039(5)	0.063(5)	0.028(5)	0.014(4)	0.000(4)	-0.004(4)
C(64)	0.045(6)	0.073(6)	0.041(6)	0.003(5)	0.011(5)	0.027(5)
C(65)	0.068(7)	0.038(4)	0.063(7)	0.003(5)	-0.011(6)	0.026(5)
C(66)	0.072(7)	0.035(4)	0.053(6)	0.001(4)	-0.001(5)	0.010(4)

Table S–11. Anisotropic Displacement Parameters for **5** (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(71)	0.034(5)	0.047(4)	0.035(5)	0.009(4)	0.012(4)	0.010(4)
C(72)	0.060(7)	0.061(5)	0.024(5)	0.003(4)	0.008(4)	0.022(5)
C(73)	0.049(7)	0.100(8)	0.045(7)	-0.016(6)	-0.002(5)	0.017(6)
C(74)	0.062(8)	0.093(8)	0.050(7)	0.013(6)	0.002(6)	0.025(7)
C(75)	0.070(9)	0.085(8)	0.091(10)	0.051(7)	0.014(7)	0.040(7)
C(76)	0.057(7)	0.045(5)	0.106(10)	0.025(6)	0.014(7)	0.004(5)
C(81)	0.062(7)	0.028(4)	0.049(6)	-0.002(4)	0.023(5)	0.009(4)
C(82)	0.065(7)	0.045(5)	0.045(6)	-0.005(4)	0.018(5)	-0.009(5)
C(83)	0.113(10)	0.046(5)	0.042(6)	0.000(5)	0.024(6)	-0.026(6)
C(84)	0.145(13)	0.053(6)	0.048(7)	-0.013(5)	0.041(8)	-0.020(7)
C(85)	0.108(11)	0.090(9)	0.060(9)	-0.005(7)	0.054(8)	0.013(8)
C(86)	0.081(8)	0.059(6)	0.068(8)	-0.019(5)	0.032(7)	-0.005(6)

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 **5**

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(5A)[a]	-0.0983	0.0660	-0.1737	0.050
H(5B)[a]	-0.0560	0.0108	-0.1441	0.050
H(5A')[b]	-0.0769	0.0161	-0.1217	0.060
H(5B')[b]	-0.1246	0.0700	-0.1545	0.060
H(6A)	-0.0350	-0.0624	-0.1023	0.039
H(6B)	-0.0688	-0.1179	-0.1266	0.039
H(7A)	-0.1901	0.1327	-0.2092	0.046
H(7B)	-0.2857	0.1531	-0.2753	0.046
H(12)	0.1227	-0.0984	-0.1411	0.065
H(13)	0.3066	-0.0981	-0.1584	0.069
H(14)	0.3617	-0.0740	-0.2856	0.066
H(15)	0.2372	-0.0471	-0.3950	0.103
H(16)	0.0562	-0.0458	-0.3769	0.096
H(22)	-0.2519	-0.0993	-0.3720	0.044
H(23)	-0.3148	-0.1743	-0.4319	0.055
H(24)	-0.2157	-0.2458	-0.4028	0.063
H(25)	-0.0534	-0.2432	-0.3151	0.075
H(26)	0.0051	-0.1688	-0.2484	0.065
H(32)	-0.4358	-0.0884	-0.1987	0.046
H(33)	-0.5281	-0.1574	-0.2586	0.067
H(34)	-0.4482	-0.2345	-0.2431	0.093
H(35)	-0.2756	-0.2437	-0.1714	0.104
H(36)	-0.1841	-0.1755	-0.1109	0.085
H(42)	-0.0843	-0.1290	0.0125	0.138
H(43)	-0.0793	-0.1416	0.1578	0.216
H(44)	-0.1791	-0.0963	0.2403	0.143
H(45)	-0.3099	-0.0446	0.1729	0.102
H(46)	-0.3241	-0.0324	0.0292	0.081
H(52)	-0.0614	0.1678	-0.2642	0.058
H(53)	0.0819	0.2099	-0.3119	0.080
H(54)	0.1357	0.1939	-0.4413	0.061
H(55)	0.0576	0.1298	-0.5203	0.110
H(56)	-0.0842	0.0861	-0.4762	0.102
H(62)	-0.3473	0.0237	-0.4390	0.046
H(63)	-0.4833	0.0368	-0.5505	0.052
H(64)	-0.5241	0.1159	-0.5997	0.063
H(65)	-0.4232	0.1821	-0.5395	0.069
H(66)	-0.2837	0.1698	-0.4346	0.065
H(72)	-0.5145	0.0214	-0.2757	0.058
H(73)	-0.6692	0.0314	-0.3686	0.078
H(74)	-0.7226	0.1090	-0.4195	0.083
H(75)	-0.6167	0.1776	-0.3723	0.098
H(76)	-0.4624	0.1684	-0.2797	0.083
H(82)	-0.2180	0.1471	-0.0715	0.061
H(83)	-0.2516	0.1905	0.0479	0.079
H(84)	-0.4216	0.1954	0.0880	0.096
H(85)	-0.5618	0.1580	0.0058	0.099
H(86)	-0.5335	0.1142	-0.1159	0.081
H(1SA)[c]	-0.2266	0.2982	0.3542	0.296
H(1SB)[c]	-0.3189	0.2608	0.3753	0.296
H(1SC)[d]	-0.2150	0.1680	0.3626	0.296
H(1SD)[d]	-0.3137	0.2029	0.3790	0.296

Table S–12. Derived Parameters for Hydrogen Atoms of **5** (continued)

[a]Included with an occupancy factor of 0.75. [b]Included with an occupancy factor of 0.25. [c]Included with an occupancy factor of 0.65. [d]Included with an occupancy factor of 0.35.

Table S-13. Crystallographic Experimental Details for **7**

A. Crystal Data	
formula	$C_{59}H_{59}BCl_4F_4IrO_3P_5Ru$
formula weight	1492.79
crystal dimensions (mm)	0.57 × 0.30 × 0.17
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	20.356 (2)
b (Å)	12.7687 (11)
c (Å)	23.221 (2)
β (deg)	91.583 (8)
V (Å^3)	6033.2 (9)
Z	4
ρ_{calcd} (g cm^{-3})	1.643
μ (mm^{-1})	9.583
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	ω
data collection 2θ limit (deg)	115.0
total data collected	7595 ($0 \le h \le 22$, $0 \le k \le 13$, $-25 \le l \le 25$)
independent reflections	7345
number of observations (*NO*)	6167 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	semiempirical (ψ scans)
range of transmission factors	0.9873–0.3069
data/restraints/parameters	7345 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 703
goodness-of-fit (S)[e]	1.074 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0659
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1739
largest difference peak and hole	2.643 and –2.124 e Å^{-3}

[a]Obtained from least-squares refinement of 44 reflections with $54.2° < 2\theta < 58.0°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Siemens.

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

(continued)

Table S-13. Crystallographic Experimental Details for **7** (continued)

[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; $w = [\sigma^2(F_o^2) + (0.1042P)^2 + 45.2444P]^{-1}$ 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-14. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **7**

(a) 'inner-core' atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Ir	0.27085(2)	0.06392(3)	0.09824(2)	0.0179(2)*
Ru	0.16918(4)	0.04507(6)	0.18201(3)	0.0185(2)*
P(1)	0.23455(13)	0.2350(2)	0.07869(11)	0.0203(6)*
P(2)	0.14365(13)	0.2246(2)	0.17796(11)	0.0203(6)*
P(3)	0.28141(12)	-0.1168(2)	0.10833(11)	0.0191(6)*
P(4)	0.20903(13)	-0.1185(2)	0.21659(11)	0.0208(6)*
P(5)	0.38474(13)	0.0970(2)	0.11045(13)	0.0254(7)*
O(1)	0.2524(4)	0.0309(7)	-0.0303(4)	0.045(2)*
O(2)	0.0910(4)	0.0464(7)	0.2905(4)	0.048(2)*
O(3)	0.0546(4)	-0.0243(7)	0.1027(3)	0.036(2)*
C(1)	0.2595(5)	0.0412(9)	0.0195(5)	0.029(3)*
C(2)	0.1214(6)	0.0472(9)	0.2491(5)	0.029(3)*
C(3)	0.0968(5)	0.0008(9)	0.1323(5)	0.026(3)*
C(4)	0.2709(6)	0.0969(12)	0.1891(5)	0.045(4)*
C(5)	0.2039(5)	0.3051(9)	0.1416(5)	0.025(3)*
C(6)	0.2859(5)	-0.1592(9)	0.1834(4)	0.022(2)*
C(7)	0.4343(6)	0.0725(11)	0.0485(5)	0.044(3)*
C(8)	0.4112(6)	0.2279(11)	0.1311(7)	0.054(4)*
C(9)	0.4282(5)	0.0248(10)	0.1655(5)	0.034(3)*

(b) dppm phenyl carbons

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(11)	0.2945(5)	0.3270(8)	0.0501(5)	0.024(3)*
C(12)	0.3122(6)	0.4189(9)	0.0786(5)	0.030(3)*
C(13)	0.3585(6)	0.4831(10)	0.0549(6)	0.038(3)*
C(14)	0.3890(7)	0.4570(10)	0.0052(6)	0.043(3)*
C(15)	0.3709(6)	0.3675(12)	-0.0226(6)	0.046(4)*
C(16)	0.3233(5)	0.2994(10)	-0.0002(5)	0.031(3)*
C(21)	0.1669(5)	0.2473(9)	0.0246(4)	0.023(2)*
C(22)	0.1198(5)	0.1682(10)	0.0186(5)	0.031(3)*
C(23)	0.0667(6)	0.1826(12)	-0.0190(5)	0.043(3)*
C(24)	0.0600(6)	0.2720(12)	-0.0513(5)	0.047(4)*
C(25)	0.1068(7)	0.3481(12)	-0.0460(6)	0.050(4)*
C(26)	0.1593(6)	0.3381(10)	-0.0076(5)	0.035(3)*
C(31)	0.1436(5)	0.2899(8)	0.2487(4)	0.023(2)*
C(32)	0.0902(6)	0.3468(10)	0.2670(5)	0.038(3)*
C(33)	0.0934(7)	0.4001(11)	0.3182(6)	0.048(4)*
C(34)	0.1494(7)	0.3952(12)	0.3533(5)	0.047(4)*
C(35)	0.2020(7)	0.3391(14)	0.3359(6)	0.064(5)*
C(36)	0.1977(6)	0.2864(11)	0.2844(5)	0.045(4)*
C(41)	0.0629(5)	0.2636(8)	0.1485(5)	0.025(3)*
C(42)	0.0087(5)	0.2030(10)	0.1632(5)	0.033(3)*
C(43)	-0.0545(5)	0.2344(11)	0.1487(5)	0.038(3)*
C(44)	-0.0644(6)	0.3285(11)	0.1184(5)	0.043(3)*
C(45)	-0.0115(6)	0.3847(11)	0.1018(6)	0.046(4)*
C(46)	0.0520(6)	0.3533(10)	0.1170(5)	0.035(3)*
C(51)	0.3535(5)	-0.1773(9)	0.0747(5)	0.025(3)*
C(52)	0.3547(5)	-0.1773(10)	0.0153(5)	0.034(3)*
C(53)	0.4070(6)	-0.2224(11)	-0.0123(6)	0.042(3)*
C(54)	0.4553(6)	-0.2711(10)	0.0184(6)	0.041(3)*
C(55)	0.4534(6)	-0.2748(10)	0.0777(6)	0.039(3)*
C(56)	0.4027(5)	-0.2302(9)	0.1065(5)	0.030(3)*
C(61)	0.2177(5)	-0.1996(9)	0.0755(5)	0.026(3)*
C(62)	0.2249(6)	-0.3083(8)	0.0804(5)	0.029(3)*
C(63)	0.1769(7)	-0.3742(10)	0.0571(5)	0.043(3)*

Table S-14. Atomic Coordinates and Displacement Parameters for **7** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C(64)	0.1250(6)	-0.3341(11)	0.0269(6)	0.045(3)*
C(65)	0.1188(5)	-0.2277(10)	0.0185(5)	0.035(3)*
C(66)	0.1650(5)	-0.1589(10)	0.0428(5)	0.035(3)*
C(71)	0.2322(5)	-0.1176(9)	0.2941(4)	0.025(3)*
C(72)	0.2406(7)	-0.2094(11)	0.3254(5)	0.047(4)*
C(73)	0.2573(8)	-0.2068(15)	0.3832(6)	0.065(5)*
C(74)	0.2668(7)	-0.1146(16)	0.4105(6)	0.063(5)*
C(75)	0.2604(7)	-0.0241(14)	0.3805(6)	0.053(4)*
C(76)	0.2434(6)	-0.0259(11)	0.3234(5)	0.039(3)*
C(81)	0.1548(5)	-0.2311(9)	0.2090(4)	0.025(3)*
C(82)	0.1802(5)	-0.3344(9)	0.2124(5)	0.034(3)*
C(83)	0.1390(7)	-0.4196(9)	0.2082(6)	0.046(4)*
C(84)	0.0719(6)	-0.4054(10)	0.1992(5)	0.036(3)*
C(85)	0.0470(6)	-0.3066(10)	0.1954(5)	0.036(3)*
C(86)	0.0887(5)	-0.2210(8)	0.2015(5)	0.023(2)*

(c) tetrafluoroborate ion atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
F(1)	0.3343(5)	-0.0927(7)	-0.3211(4)	0.073(3)*
F(2)	0.3375(11)	0.0665(9)	-0.2844(6)	0.171(8)*
F(3)	0.3271(8)	-0.0678(12)	-0.2269(5)	0.143(6)*
F(4)	0.4179(6)	-0.0364(15)	-0.2664(8)	0.167(7)*
B	0.3547(9)	-0.0357(15)	-0.2748(9)	0.058(5)*

(d) solvent dichloromethane atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Cl(1)	0.3993(3)	0.1108(4)	-0.1098(2)	0.098(2)*
Cl(2)	0.3804(3)	0.2932(5)	-0.1830(2)	0.102(2)*
C(91)	0.4076(14)	0.1660(19)	-0.1764(9)	0.130(10)*
Cl(3)	0.4654(4)	0.5613(5)	-0.1174(3)	0.130(2)*
Cl(4)	0.4343(3)	0.6948(5)	-0.2160(3)	0.117(2)*
C(92)	0.4520(18)	0.5694(18)	-0.1838(10)	0.168(16)*

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-15. Selected Interatomic Distances (Å) for **7**

(a) involving 'inner-core' atoms

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Ir	Ru	2.8892(9)	P(1)	C(5)	1.837(11)
Ir	P(1)	2.347(3)	P(2)	C(5)	1.824(10)
Ir	P(3)	2.329(3)	P(3)	C(6)	1.826(10)
Ir	P(5)	2.366(3)	P(4)	C(6)	1.838(10)
Ir	C(1)	1.859(12)	P(5)	C(7)	1.807(13)
Ir	C(4)	2.152(11)	P(5)	C(8)	1.816(13)
Ru	P(2)	2.352(3)	P(5)	C(9)	1.790(11)
Ru	P(4)	2.373(3)	O(1)	C(1)	1.168(13)
Ru	C(2)	1.859(13)	O(2)	C(2)	1.159(14)
Ru	C(3)	1.931(11)	O(3)	C(3)	1.133(12)
Ru	C(4)	2.175(13)			

(b) involving dppm phenyl carbons

Atom1	Atom2	Distance	Atom1	Atom2	Distance
P(1)	C(11)	1.832(10)	C(42)	C(43)	1.38(2)
P(1)	C(21)	1.843(10)	C(43)	C(44)	1.40(2)
P(2)	C(31)	1.841(10)	C(44)	C(45)	1.36(2)
P(2)	C(41)	1.832(10)	C(45)	C(46)	1.39(2)
P(3)	C(51)	1.850(10)	C(51)	C(52)	1.38(2)
P(3)	C(61)	1.823(11)	C(51)	C(56)	1.402(15)
P(4)	C(71)	1.848(10)	C(52)	C(53)	1.38(2)
P(4)	C(81)	1.818(11)	C(53)	C(54)	1.35(2)
C(11)	C(12)	1.39(2)	C(54)	C(55)	1.38(2)
C(11)	C(16)	1.37(2)	C(55)	C(56)	1.37(2)
C(12)	C(13)	1.38(2)	C(61)	C(62)	1.40(2)
C(13)	C(14)	1.37(2)	C(61)	C(66)	1.40(2)
C(14)	C(15)	1.36(2)	C(62)	C(63)	1.39(2)
C(15)	C(16)	1.41(2)	C(63)	C(64)	1.35(2)
C(21)	C(22)	1.40(2)	C(64)	C(65)	1.38(2)
C(21)	C(26)	1.39(2)	C(65)	C(66)	1.39(2)
C(22)	C(23)	1.38(2)	C(71)	C(72)	1.39(2)
C(23)	C(24)	1.37(2)	C(71)	C(76)	1.37(2)
C(24)	C(25)	1.37(2)	C(72)	C(73)	1.38(2)
C(25)	C(26)	1.38(2)	C(73)	C(74)	1.35(2)
C(31)	C(32)	1.38(2)	C(74)	C(75)	1.35(2)
C(31)	C(36)	1.36(2)	C(75)	C(76)	1.36(2)
C(32)	C(33)	1.37(2)	C(81)	C(82)	1.42(2)
C(33)	C(34)	1.38(2)	C(81)	C(86)	1.359(15)
C(34)	C(35)	1.36(2)	C(82)	C(83)	1.37(2)
C(35)	C(36)	1.37(2)	C(83)	C(84)	1.39(2)
C(41)	C(42)	1.40(2)	C(84)	C(85)	1.36(2)
C(41)	C(46)	1.37(2)	C(85)	C(86)	1.39(2)

(c) within the teterafluoroborate ion

Atom1	Atom2	Distance	Atom1	Atom2	Distance
F(1)	B	1.36(2)	F(3)	B	1.32(2)
F(2)	B	1.37(2)	F(4)	B	1.30(2)

(d) within the solvent dichloromethane molecules

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Cl(1)	C(91)	1.71(2)	Cl(3)	C(92)	1.56(2)
Cl(2)	C(91)	1.72(2)	Cl(4)	C(92)	1.80(2)

Table S-16. Selected Interatomic Angles (deg) for **7**

(a) involving 'inner-core' atoms

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ru	Ir	P(1)	88.87(7)	P(2)	Ru	C(4)	85.1(4)
Ru	Ir	P(3)	85.16(7)	P(4)	Ru	C(2)	84.9(3)
Ru	Ir	P(5)	130.69(7)	P(4)	Ru	C(3)	101.1(4)
Ru	Ir	C(1)	125.3(3)	P(4)	Ru	C(4)	85.8(4)
Ru	Ir	C(4)	48.5(3)	C(2)	Ru	C(3)	95.6(5)
P(1)	Ir	P(3)	165.86(9)	C(2)	Ru	C(4)	116.8(5)
P(1)	Ir	P(5)	99.15(10)	C(3)	Ru	C(4)	147.5(4)
P(1)	Ir	C(1)	85.7(4)	Ir	P(1)	C(5)	114.3(4)
P(1)	Ir	C(4)	89.9(4)	Ru	P(2)	C(5)	114.6(4)
P(3)	Ir	P(5)	94.45(9)	Ir	P(3)	C(6)	113.1(4)
P(3)	Ir	C(1)	87.3(4)	Ru	P(4)	C(6)	113.2(4)
P(3)	Ir	C(4)	95.6(4)	Ir	P(5)	C(7)	116.2(4)
P(5)	Ir	C(1)	103.9(3)	Ir	P(5)	C(8)	118.6(4)
P(5)	Ir	C(4)	82.8(3)	Ir	P(5)	C(9)	117.2(4)
C(1)	Ir	C(4)	172.6(4)	C(7)	P(5)	C(8)	101.6(7)
Ir	Ru	P(2)	93.06(7)	C(7)	P(5)	C(9)	101.7(6)
Ir	Ru	P(4)	93.25(7)	C(8)	P(5)	C(9)	98.5(6)
Ir	Ru	C(2)	164.5(4)	Ir	C(1)	O(1)	177.5(11)
Ir	Ru	C(3)	99.8(3)	Ru	C(2)	O(2)	178.4(11)
Ir	Ru	C(4)	47.8(3)	Ru	C(3)	O(3)	179.2(9)
P(2)	Ru	P(4)	160.86(10)	Ir	C(4)	Ru	83.8(5)
P(2)	Ru	C(2)	84.2(3)	P(1)	C(5)	P(2)	110.0(6)
P(2)	Ru	C(3)	95.6(4)	P(3)	C(6)	P(4)	107.2(5)

(b) involving dppm phenyl carbons

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Ir	P(1)	C(11)	117.2(4)	P(1)	C(21)	C(26)	120.6(9)
Ir	P(1)	C(21)	115.8(4)	C(22)	C(21)	C(26)	118.9(10)
C(5)	P(1)	C(11)	102.8(5)	C(21)	C(22)	C(23)	119.4(12)
C(5)	P(1)	C(21)	103.7(5)	C(22)	C(23)	C(24)	121.3(13)
C(11)	P(1)	C(21)	101.0(5)	C(23)	C(24)	C(25)	119.0(12)
Ru	P(2)	C(31)	114.3(3)	C(24)	C(25)	C(26)	121.2(13)
Ru	P(2)	C(41)	118.3(4)	C(21)	C(26)	C(25)	120.0(12)
C(5)	P(2)	C(31)	100.1(5)	P(2)	C(31)	C(32)	122.1(9)
C(5)	P(2)	C(41)	106.4(5)	P(2)	C(31)	C(36)	120.5(8)
C(31)	P(2)	C(41)	100.8(5)	C(32)	C(31)	C(36)	117.3(10)
Ir	P(3)	C(51)	116.3(4)	C(31)	C(32)	C(33)	120.6(12)
Ir	P(3)	C(61)	118.0(4)	C(32)	C(33)	C(34)	120.4(13)
C(6)	P(3)	C(51)	105.1(5)	C(33)	C(34)	C(35)	119.5(12)
C(6)	P(3)	C(61)	104.1(5)	C(34)	C(35)	C(36)	119.0(13)
C(51)	P(3)	C(61)	98.3(5)	C(31)	C(36)	C(35)	123.1(12)
Ru	P(4)	C(71)	113.6(4)	P(2)	C(41)	C(42)	117.7(8)
Ru	P(4)	C(81)	117.5(4)	P(2)	C(41)	C(46)	123.7(9)
C(6)	P(4)	C(71)	102.2(5)	C(42)	C(41)	C(46)	118.4(10)
C(6)	P(4)	C(81)	104.9(5)	C(41)	C(42)	C(43)	121.0(12)
C(71)	P(4)	C(81)	103.8(5)	C(42)	C(43)	C(44)	119.4(12)
P(1)	C(11)	C(12)	122.3(8)	C(43)	C(44)	C(45)	119.4(11)
P(1)	C(11)	C(16)	116.7(9)	C(44)	C(45)	C(46)	120.9(13)
C(12)	C(11)	C(16)	120.9(10)	C(41)	C(46)	C(45)	120.7(12)
C(11)	C(12)	C(13)	118.9(11)	P(3)	C(51)	C(52)	117.3(8)
C(12)	C(13)	C(14)	121.7(12)	P(3)	C(51)	C(56)	122.9(8)
C(13)	C(14)	C(15)	118.9(12)	C(52)	C(51)	C(56)	119.6(10)
C(14)	C(15)	C(16)	121.5(13)	C(51)	C(52)	C(53)	120.0(11)
C(11)	C(16)	C(15)	118.1(12)	C(52)	C(53)	C(54)	120.2(12)
P(1)	C(21)	C(22)	120.3(8)	C(53)	C(54)	C(55)	120.2(11)

Table S-16. Selected Interatomic Angles for **7** (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C(54)	C(55)	C(56)	121.1(11)	C(71)	C(72)	C(73)	120.9(14)
C(51)	C(56)	C(55)	118.7(11)	C(72)	C(73)	C(74)	120.5(15)
P(3)	C(61)	C(62)	118.0(8)	C(73)	C(74)	C(75)	119.5(13)
P(3)	C(61)	C(66)	122.6(9)	C(74)	C(75)	C(76)	120.4(15)
C(62)	C(61)	C(66)	119.3(10)	C(71)	C(76)	C(75)	122.2(13)
C(61)	C(62)	C(63)	119.9(11)	P(4)	C(81)	C(82)	120.7(8)
C(62)	C(63)	C(64)	120.4(12)	P(4)	C(81)	C(86)	122.3(8)
C(63)	C(64)	C(65)	120.8(12)	C(82)	C(81)	C(86)	117.0(10)
C(64)	C(65)	C(66)	120.4(11)	C(81)	C(82)	C(83)	120.7(11)
C(61)	C(66)	C(65)	119.0(12)	C(82)	C(83)	C(84)	120.2(12)
P(4)	C(71)	C(72)	121.9(9)	C(83)	C(84)	C(85)	119.5(11)
P(4)	C(71)	C(76)	121.6(9)	C(84)	C(85)	C(86)	119.9(11)
C(72)	C(71)	C(76)	116.5(10)	C(81)	C(86)	C(85)	122.6(11)

(c) within the teterafluoroborate ion

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
F(1)	B	F(2)	108.2(14)	F(2)	B	F(3)	108.6(19)
F(1)	B	F(3)	111.9(15)	F(2)	B	F(4)	106.2(17)
F(1)	B	F(4)	113.4(18)	F(3)	B	F(4)	108.4(17)

(d) within the solvent dichloromethane molecules

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Cl(1)	C(91)	Cl(2)	115.4(12)	Cl(3)	C(92)	Cl(4)	119.8(13)

Table S-17. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **7**

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir	0.0140(3)	0.0159(3)	0.0237(3)	0.0005(2)	-0.0015(2)	0.0004(2)
Ru	0.0144(4)	0.0155(5)	0.0256(5)	0.0004(3)	0.0002(3)	0.0003(3)
P(1)	0.0192(14)	0.0149(15)	0.0268(14)	0.0034(12)	-0.0006(11)	0.0005(12)
P(2)	0.0179(13)	0.0170(15)	0.0260(14)	-0.0014(12)	0.0000(11)	0.0005(12)
P(3)	0.0150(13)	0.0174(15)	0.0248(14)	0.0005(11)	-0.0010(11)	0.0002(12)
P(4)	0.0174(13)	0.020(2)	0.0252(14)	0.0027(12)	0.0008(11)	0.0016(12)
P(5)	0.0168(13)	0.021(2)	0.038(2)	0.0045(13)	-0.0053(12)	-0.0056(12)
O(1)	0.051(6)	0.053(6)	0.029(5)	0.007(4)	0.003(4)	0.003(5)
O(2)	0.043(5)	0.054(6)	0.047(6)	0.004(5)	0.022(5)	0.011(5)
O(3)	0.022(4)	0.044(5)	0.041(5)	-0.002(4)	-0.005(4)	-0.010(4)
C(1)	0.024(6)	0.032(7)	0.029(7)	0.006(5)	-0.001(5)	0.000(5)
C(2)	0.027(6)	0.019(6)	0.041(7)	0.003(5)	0.000(6)	0.011(5)
C(3)	0.016(6)	0.029(7)	0.032(6)	0.003(5)	0.002(5)	-0.006(5)
C(4)	0.032(7)	0.082(11)	0.020(6)	0.008(7)	0.012(5)	0.041(7)
C(5)	0.026(6)	0.013(6)	0.037(6)	-0.002(5)	0.010(5)	-0.007(5)
C(6)	0.013(5)	0.029(7)	0.026(6)	-0.002(5)	-0.002(4)	0.013(5)
C(7)	0.033(7)	0.061(10)	0.038(7)	0.008(7)	0.003(6)	-0.006(7)
C(8)	0.025(7)	0.042(9)	0.092(11)	-0.003(8)	-0.028(7)	-0.011(6)
C(9)	0.023(6)	0.038(8)	0.040(7)	0.008(6)	-0.008(5)	-0.003(6)
C(11)	0.018(5)	0.017(6)	0.036(7)	0.008(5)	0.003(5)	-0.001(5)
C(12)	0.029(6)	0.021(7)	0.041(7)	0.015(6)	0.007(5)	0.000(6)
C(13)	0.044(8)	0.021(7)	0.051(8)	-0.005(6)	0.008(7)	-0.003(6)
C(14)	0.045(8)	0.025(7)	0.058(9)	0.012(7)	0.007(7)	-0.008(6)
C(15)	0.030(7)	0.063(10)	0.044(8)	0.020(7)	0.003(6)	0.000(7)
C(16)	0.033(7)	0.032(7)	0.028(6)	0.005(5)	-0.009(5)	0.003(6)
C(21)	0.021(6)	0.024(6)	0.025(6)	0.001(5)	-0.007(5)	0.008(5)
C(22)	0.026(6)	0.030(7)	0.037(7)	0.002(6)	-0.005(5)	0.008(6)
C(23)	0.032(7)	0.059(9)	0.037(7)	-0.011(7)	-0.007(6)	-0.003(7)
C(24)	0.035(7)	0.071(11)	0.035(7)	-0.002(7)	-0.012(6)	0.007(8)
C(25)	0.051(8)	0.051(9)	0.046(8)	0.020(7)	-0.005(7)	0.024(8)
C(26)	0.037(7)	0.027(7)	0.040(7)	0.002(6)	-0.006(6)	0.013(6)
C(31)	0.030(6)	0.013(6)	0.026(6)	-0.003(5)	-0.002(5)	-0.001(5)
C(32)	0.039(7)	0.031(7)	0.046(8)	-0.003(6)	0.004(6)	-0.004(6)
C(33)	0.047(8)	0.046(9)	0.052(8)	-0.027(7)	0.007(7)	-0.001(7)
C(34)	0.051(8)	0.062(10)	0.028(7)	-0.016(7)	0.005(6)	-0.010(8)
C(35)	0.045(8)	0.090(13)	0.055(9)	-0.033(9)	-0.021(7)	0.013(9)
C(36)	0.043(8)	0.049(9)	0.042(7)	-0.025(7)	-0.006(6)	0.021(7)
C(41)	0.029(6)	0.013(6)	0.034(6)	-0.010(5)	-0.004(5)	0.015(5)
C(42)	0.018(6)	0.048(8)	0.033(6)	-0.006(6)	0.001(5)	0.010(6)
C(43)	0.020(6)	0.048(9)	0.047(7)	-0.006(7)	-0.004(5)	-0.009(6)
C(44)	0.029(7)	0.054(9)	0.046(8)	0.000(7)	-0.011(6)	0.013(7)
C(45)	0.040(8)	0.047(9)	0.051(8)	-0.007(7)	-0.015(7)	0.021(7)
C(46)	0.028(6)	0.031(7)	0.045(7)	0.000(6)	-0.001(6)	0.012(6)
C(51)	0.016(5)	0.019(6)	0.038(7)	-0.002(5)	0.010(5)	-0.003(5)
C(52)	0.023(6)	0.049(8)	0.030(7)	-0.004(6)	-0.001(5)	0.008(6)
C(53)	0.044(8)	0.045(8)	0.038(7)	-0.003(6)	0.010(6)	0.001(7)
C(54)	0.020(6)	0.031(7)	0.073(10)	-0.003(7)	0.023(6)	-0.003(6)
C(55)	0.021(6)	0.029(7)	0.067(9)	0.004(7)	0.001(6)	0.006(6)
C(56)	0.016(6)	0.026(7)	0.047(7)	-0.002(6)	-0.004(5)	0.007(5)
C(61)	0.022(6)	0.032(7)	0.025(6)	-0.004(5)	0.006(5)	-0.007(5)
C(62)	0.031(6)	0.014(6)	0.039(7)	-0.005(5)	-0.013(5)	0.001(5)
C(63)	0.057(9)	0.028(7)	0.045(8)	-0.003(6)	0.001(7)	-0.009(7)
C(64)	0.036(7)	0.044(9)	0.054(8)	-0.004(7)	-0.007(6)	-0.015(7)
C(65)	0.022(6)	0.033(8)	0.048(7)	-0.007(6)	-0.009(5)	-0.003(6)
C(66)	0.017(6)	0.040(8)	0.049(8)	-0.004(6)	0.009(5)	0.005(6)

Table S-17. Anisotropic Displacement Parameters for **7** (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(71)	0.019(5)	0.035(7)	0.021(6)	0.003(5)	-0.006(5)	0.007(5)
C(72)	0.063(9)	0.043(9)	0.035(7)	0.002(6)	-0.013(6)	0.017(7)
C(73)	0.072(11)	0.078(13)	0.044(9)	0.027(9)	-0.004(8)	0.005(10)
C(74)	0.053(9)	0.112(16)	0.023(7)	0.007(9)	-0.007(7)	0.009(10)
C(75)	0.047(8)	0.079(12)	0.032(7)	-0.010(8)	-0.010(6)	0.000(8)
C(76)	0.041(7)	0.052(9)	0.022(6)	0.001(6)	-0.010(5)	0.002(7)
C(81)	0.029(6)	0.019(6)	0.028(6)	0.000(5)	-0.001(5)	-0.008(5)
C(82)	0.021(6)	0.024(7)	0.057(8)	-0.003(6)	0.014(6)	0.004(6)
C(83)	0.048(8)	0.012(7)	0.081(10)	0.002(6)	0.027(7)	-0.001(6)
C(84)	0.034(7)	0.030(7)	0.046(8)	-0.001(6)	0.009(6)	-0.009(6)
C(85)	0.032(7)	0.044(9)	0.034(7)	-0.013(6)	0.008(5)	-0.004(6)
C(86)	0.026(6)	0.006(6)	0.037(6)	0.002(5)	0.003(5)	-0.006(5)
F(1)	0.089(7)	0.053(6)	0.077(6)	-0.015(5)	0.012(5)	-0.030(5)
F(2)	0.342(25)	0.067(9)	0.100(9)	-0.031(7)	-0.094(13)	0.025(11)
F(3)	0.197(15)	0.166(14)	0.067(7)	0.011(8)	0.009(8)	-0.078(11)
F(4)	0.074(9)	0.212(18)	0.214(17)	-0.049(14)	-0.021(10)	-0.027(10)
B	0.058(11)	0.047(12)	0.069(13)	0.000(9)	-0.022(10)	-0.012(9)
Cl(1)	0.109(4)	0.092(4)	0.091(3)	-0.013(3)	0.002(3)	0.005(3)
Cl(2)	0.109(4)	0.107(4)	0.089(3)	-0.007(3)	-0.024(3)	0.004(3)
C(91)	0.194(27)	0.121(21)	0.073(14)	-0.040(14)	-0.009(15)	0.062(19)
Cl(3)	0.201(7)	0.109(5)	0.082(4)	0.002(3)	0.031(4)	-0.029(5)
Cl(4)	0.118(4)	0.101(4)	0.126(4)	-0.005(4)	-0.069(4)	0.006(4)
C(92)	0.306(43)	0.091(18)	0.102(18)	-0.044(15)	-0.090(23)	0.079(22)

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-18. Derived Parameters for Hydrogen Atoms of **7**

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(4A)	0.2765	0.1710	0.1991	0.054
H(4B)	0.2997	0.0518	0.2127	0.054
H(5A)	0.2406	0.3214	0.1683	0.030
H(5B)	0.1835	0.3712	0.1292	0.030
H(6A)	0.3237	-0.1267	0.2035	0.027
H(6B)	0.2909	-0.2354	0.1856	0.027
H(7A)	0.4153	0.1084	0.0152	0.053
H(7B)	0.4357	-0.0021	0.0410	0.053
H(7C)	0.4786	0.0982	0.0561	0.053
H(8A)	0.3915	0.2786	0.1048	0.064
H(8B)	0.4587	0.2323	0.1296	0.064
H(8C)	0.3976	0.2425	0.1700	0.064
H(9A)	0.4058	0.0321	0.2016	0.041
H(9B)	0.4726	0.0518	0.1699	0.041
H(9C)	0.4297	-0.0486	0.1548	0.041
H(12)	0.2927	0.4370	0.1135	0.036
H(13)	0.3695	0.5465	0.0733	0.046
H(14)	0.4220	0.5003	-0.0095	0.051
H(15)	0.3906	0.3505	-0.0576	0.055
H(16)	0.3117	0.2369	-0.0193	0.038
H(22)	0.1241	0.1059	0.0399	0.037
H(23)	0.0345	0.1300	-0.0224	0.051
H(24)	0.0236	0.2807	-0.0767	0.057
H(25)	0.1032	0.4085	-0.0690	0.060
H(26)	0.1899	0.3929	-0.0032	0.042
H(32)	0.0515	0.3489	0.2441	0.046
H(33)	0.0573	0.4402	0.3296	0.058
H(34)	0.1510	0.4302	0.3889	0.056
H(35)	0.2409	0.3366	0.3587	0.076
H(36)	0.2338	0.2460	0.2733	0.054
H(42)	0.0154	0.1399	0.1834	0.040
H(43)	-0.0906	0.1931	0.1589	0.046
H(44)	-0.1073	0.3524	0.1098	0.052
H(45)	-0.0180	0.4456	0.0796	0.056
H(46)	0.0879	0.3940	0.1057	0.042
H(52)	0.3201	-0.1466	-0.0063	0.041
H(53)	0.4088	-0.2193	-0.0527	0.051
H(54)	0.4903	-0.3026	-0.0006	0.049
H(55)	0.4874	-0.3084	0.0986	0.047
H(56)	0.4009	-0.2351	0.1468	0.035
H(62)	0.2622	-0.3367	0.0994	0.034
H(63)	0.1805	-0.4470	0.0623	0.052
H(64)	0.0927	-0.3795	0.0114	0.054
H(65)	0.0832	-0.2012	-0.0037	0.042
H(66)	0.1607	-0.0863	0.0372	0.042
H(72)	0.2348	-0.2743	0.3068	0.057
H(73)	0.2621	-0.2698	0.4038	0.078
H(74)	0.2778	-0.1132	0.4501	0.075
H(75)	0.2677	0.0403	0.3992	0.064
H(76)	0.2391	0.0379	0.3035	0.047
H(82)	0.2257	-0.3448	0.2176	0.040
H(83)	0.1564	-0.4876	0.2113	0.056
H(84)	0.0438	-0.4636	0.1959	0.043
H(85)	0.0017	-0.2963	0.1887	0.044
H(86)	0.0705	-0.1534	0.2003	0.028

Table S-18. Derived Parameters for Hydrogen Atoms of **7** (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H(91A)	0.3835	0.1229	-0.2048	0.156
H(91B)	0.4542	0.1640	-0.1861	0.156
H(92A)	0.4149	0.5231	-0.1935	0.202
H(92B)	0.4905	0.5408	-0.2028	0.202