Electronic Supplementary Information for Dalton Transactions

C-H activation on a diphosphine and hydrido-bridged diiridium complex. Generation and detection of an active Ir^{II}-Ir^{II} species $[(Cp^*Ir)_2(\mu\text{-dmpm})(\mu\text{-H})]^+$

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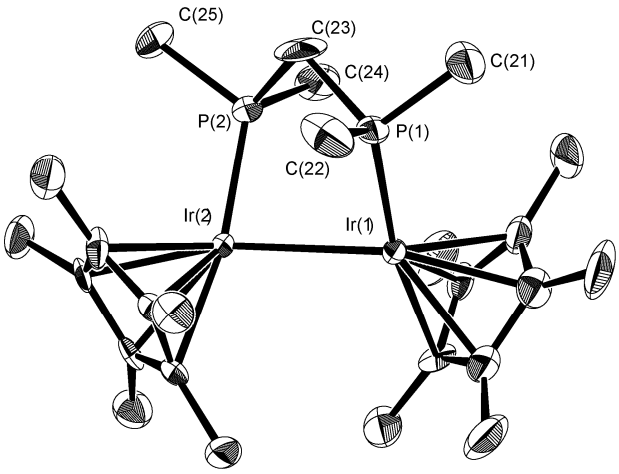
Electronic Supplementary Information: List of crystal data and structure refinement, atomic coordinates, bond lengths, angles etc.

Details of the X-ray crystal structures for complex 3



A. Crystal Data

Empirical Formula	$C_{25}H_{46}Ir_2P_2$
Formula Weight	793.03
Crystal Color, Habit	orange, block
Crystal Dimensions	0.60 X 0.50 X 0.30 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2θ range)	24 (29.5 - 29.9^o)
Omega Scan Peak Width	
at Half-height	0.17^o
Lattice Parameters	a = 8.505(6) Å
	b = 16.341(7) Å
	c = 20.088(4) Å
	β = 96.95(3) ^{o}
	V = 2771.2(23) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.901 g/cm^3
F_{000}	1520.00

μ(MoKα)	97.461 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5S
Radiation	MoKα (λ = 0.71069 Å)
	graphite monochromated
Attenuator	Zr foil (factors = 1.00, 2.24, 5.29, 11.80)
Take-off Angle	6.0^o
Detector Aperture	13.0 mm horizontal
	9.0 mm vertical
Crystal to Detector Distance	258 mm
Voltage, Current	50 kV, 20 mA
Temperature	-70.0^oC
Scan Type	ω-2θ
Scan Rate	2.0^o/min (in ω)
Scan Width	$(1.26 + 0.30 \tan \theta)^o$
$2\theta_{max}$	55.0^o
No. of Reflections Measured	Total: 6744
	Unique: 6213 (R_{int} = 0.064)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.023 - 0.054)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF99 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	$\Sigma w (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/[0.0048Fo^2+1.0000\sigma(Fo^2)]$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	5326
No. Variables	306
Reflection/Parameter Ratio	17.41

Residuals: R (I>3.00σ(I))	0.0447
Residuals: Rw (I>3.00σ(I))	0.0738
Goodness of Fit Indicator	1.004
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	3.54 $e^-/Å^3$
Minimum peak in Final Diff. Map	-4.36 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ir(1)	0.79117(3)	0.74445(2)	0.424620(10)	1.450(7)
Ir(2)	0.59345(3)	0.81746(2)	0.322460(10)	1.379(7)
P(1)	0.9088(2)	0.68521(13)	0.34563(12)	1.98(4)
P(2)	0.5846(2)	0.69586(13)	0.27593(12)	2.20(4)
C(1)	0.7502(10)	0.6449(6)	0.5012(4)	2.49(17)
C(2)	0.6148(10)	0.6948(5)	0.4940(4)	2.19(17)
C(3)	0.6544(11)	0.7756(6)	0.5116(4)	2.59(18)
C(4)	0.8189(13)	0.7778(6)	0.5337(5)	3.2(2)
C(5)	0.8837(11)	0.6976(6)	0.5269(5)	2.9(2)
C(6)	0.7582(18)	0.5544(6)	0.4957(5)	4.9(3)
C(7)	0.4463(13)	0.6651(8)	0.4782(5)	4.3(2)
C(8)	0.5390(14)	0.8436(7)	0.5157(5)	3.9(2)
C(9)	0.9129(16)	0.8475(8)	0.5629(5)	4.7(3)
C(10)	1.0436(17)	0.6682(10)	0.5505(6)	5.7(3)
C(11)	0.4697(8)	0.9386(4)	0.3212(4)	1.75(14)
C(12)	0.4652(10)	0.9092(4)	0.2530(4)	2.12(15)
C(13)	0.6308(10)	0.9068(5)	0.2389(4)	2.52(18)
C(14)	0.7287(9)	0.9333(4)	0.2958(4)	1.98(15)
C(15)	0.6281(9)	0.9518(4)	0.3476(4)	1.82(14)
C(16)	0.3296(11)	0.9567(6)	0.3572(5)	3.1(2)
C(17)	0.3201(12)	0.8965(6)	0.2036(5)	3.2(2)
C(18)	0.6770(14)	0.8925(7)	0.1700(5)	4.1(2)
C(19)	0.9010(11)	0.9525(6)	0.3005(5)	3.2(2)
C(20)	0.6940(12)	0.9924(6)	0.4123(5)	3.4(2)
C(21)	1.0260(14)	0.5937(7)	0.3671(5)	3.9(2)
C(22)	1.0577(17)	0.7436(7)	0.3089(7)	4.7(3)
C(23)	0.7765(14)	0.6481(7)	0.2702(5)	4.1(2)
C(24)	0.4858(16)	0.6131(6)	0.3159(6)	4.4(2)
C(25)	0.4956(19)	0.6877(7)	0.1884(6)	5.1(3)

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.6578	0.5331	0.4779	5.96
H(2)	0.7889	0.5315	0.5388	5.95
H(3)	0.8345	0.5406	0.4667	5.96
H(4)	0.3743	0.7093	0.4798	5.32
H(5)	0.4269	0.6252	0.5107	5.32
H(6)	0.4323	0.6411	0.4349	5.32
H(7)	0.5931	0.8910	0.5338	4.86
H(8)	0.4623	0.8275	0.5438	4.86
H(9)	0.4878	0.8555	0.4721	4.86
H(10)	1.0188	0.8306	0.5764	5.56
H(11)	0.8676	0.8675	0.6007	5.56
H(12)	0.9124	0.8896	0.5303	5.56
H(13)	1.0501	0.6111	0.5424	6.68
H(14)	1.0667	0.6784	0.5972	6.68
H(15)	1.1179	0.6962	0.5271	6.68
H(16)	0.2346	0.9452	0.3287	3.80
H(17)	0.3313	1.0128	0.3695	3.81
H(18)	0.3342	0.9237	0.3963	3.80
H(19)	0.3493	0.8796	0.1615	3.74
H(20)	0.2623	0.9463	0.1981	3.74
H(21)	0.2562	0.8555	0.2203	3.74
H(22)	0.7890	0.8959	0.1723	4.86
H(23)	0.6299	0.9330	0.1400	4.86
H(24)	0.6428	0.8398	0.1543	4.86
H(25)	0.9348	0.9756	0.3432	3.86
H(26)	0.9192	0.9905	0.2664	3.85
H(27)	0.9589	0.9037	0.2951	3.86
H(28)	0.6103	1.0030	0.4384	3.98
H(29)	0.7434	1.0425	0.4028	3.98
H(30)	0.7696	0.9574	0.4365	3.98

H(31)	1.1325	0.6084	0.3821	4.85
H(32)	1.0235	0.5599	0.3285	4.84
H(33)	0.9826	0.5648	0.4016	4.85
H(34)	1.0086	0.7732	0.2713	5.93
H(35)	1.1347	0.7074	0.2949	5.93
H(36)	1.1075	0.7808	0.3412	5.93
H(37)	0.8166	0.6657	0.2304	5.02
H(38)	0.7681	0.5901	0.2700	5.00
H(39)	0.5602	0.5858	0.3474	5.25
H(40)	0.4415	0.5752	0.2830	5.24
H(41)	0.4039	0.6358	0.3384	5.25
H(42)	0.3852	0.6775	0.1867	5.72
H(43)	0.5443	0.6438	0.1675	5.72
H(44)	0.5119	0.7373	0.1655	5.72

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.0207(2)	0.01969(19)	0.0145(2)	0.00453(10)	0.00120(13)	-0.00027(10)
Ir(2)	0.02192(19)	0.01628(18)	0.01343(19)	0.00029(10)	-0.00094(12)	-0.00016(10)
P(1)	0.0269(10)	0.0256(10)	0.0242(11)	0.0063(7)	0.0098(8)	-0.0022(8)
P(2)	0.0364(11)	0.0226(9)	0.0228(11)	0.0019(8)	-0.0037(9)	-0.0053(8)
C(1)	0.033(4)	0.040(4)	0.020(4)	0.008(3)	-0.002(3)	0.005(3)
C(2)	0.031(4)	0.037(4)	0.016(4)	0.000(3)	0.008(3)	0.009(3)
C(3)	0.043(5)	0.044(5)	0.014(4)	0.010(4)	0.019(3)	-0.007(3)
C(4)	0.060(6)	0.035(5)	0.025(5)	-0.001(4)	0.001(4)	0.003(4)
C(5)	0.027(4)	0.048(5)	0.035(5)	0.011(3)	0.004(3)	0.002(4)
C(6)	0.111(10)	0.045(6)	0.033(5)	0.022(6)	0.025(6)	0.021(5)
C(7)	0.048(6)	0.087(8)	0.034(6)	-0.017(6)	0.018(4)	0.010(6)
C(8)	0.065(7)	0.058(6)	0.031(5)	0.026(5)	0.021(5)	0.005(5)
C(9)	0.076(8)	0.074(8)	0.026(5)	-0.007(7)	-0.009(5)	-0.008(5)
C(10)	0.072(8)	0.113(12)	0.027(6)	0.044(8)	-0.007(5)	0.016(6)
C(11)	0.017(3)	0.014(3)	0.035(4)	0.007(2)	0.001(2)	0.008(3)
C(12)	0.037(4)	0.015(3)	0.027(4)	0.006(3)	-0.006(3)	0.011(3)
C(13)	0.036(4)	0.035(4)	0.024(4)	0.006(3)	0.002(3)	0.015(3)
C(14)	0.033(4)	0.016(3)	0.026(4)	0.001(3)	0.000(3)	0.002(3)
C(15)	0.031(3)	0.011(3)	0.026(4)	0.001(2)	0.002(3)	0.002(2)
C(16)	0.042(5)	0.037(5)	0.041(5)	0.004(4)	0.012(4)	0.002(4)
C(17)	0.044(5)	0.045(5)	0.030(5)	0.001(4)	-0.015(4)	0.005(4)
C(18)	0.063(7)	0.057(6)	0.033(5)	0.018(5)	0.004(5)	0.008(5)
C(19)	0.037(4)	0.039(5)	0.045(6)	-0.004(4)	0.009(4)	0.003(4)
C(20)	0.052(5)	0.038(5)	0.036(5)	0.014(4)	-0.015(4)	-0.012(4)
C(21)	0.063(6)	0.048(6)	0.042(6)	0.023(5)	0.024(5)	0.008(5)
C(22)	0.075(8)	0.038(6)	0.074(9)	0.007(5)	0.049(7)	0.007(5)
C(23)	0.065(7)	0.056(6)	0.038(6)	0.012(5)	0.020(5)	-0.030(5)
C(24)	0.097(9)	0.027(5)	0.043(6)	-0.021(5)	-0.001(6)	-0.007(4)
C(25)	0.101(10)	0.045(6)	0.036(6)	0.002(6)	-0.040(7)	-0.016(4)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ir(1)	Ir(2)	2.7618(3)	Ir(1)	P(1)	2.200(2)
Ir(1)	C(1)	2.295(9)	Ir(1)	C(2)	2.314(9)
Ir(1)	C(3)	2.271(9)	Ir(1)	C(4)	2.243(10)
Ir(1)	C(5)	2.244(10)	Ir(2)	P(2)	2.193(2)
Ir(2)	C(11)	2.241(7)	Ir(2)	C(12)	2.239(7)
Ir(2)	C(13)	2.276(9)	Ir(2)	C(14)	2.311(8)
Ir(2)	C(15)	2.263(7)	P(1)	C(21)	1.819(11)
P(1)	C(22)	1.812(14)	P(1)	C(23)	1.876(11)
P(2)	C(23)	1.825(12)	P(2)	C(24)	1.828(12)
P(2)	C(25)	1.834(12)	C(1)	C(2)	1.405(12)
C(1)	C(5)	1.469(13)	C(1)	C(6)	1.485(14)
C(2)	C(3)	1.397(13)	C(2)	C(7)	1.510(14)
C(3)	C(4)	1.416(14)	C(3)	C(8)	1.492(16)
C(4)	C(5)	1.434(14)	C(4)	C(9)	1.471(17)
C(5)	C(10)	1.466(17)	C(11)	C(12)	1.449(12)
C(11)	C(15)	1.404(10)	C(11)	C(16)	1.496(13)
C(12)	C(13)	1.470(12)	C(12)	C(17)	1.501(12)
C(13)	C(14)	1.398(11)	C(13)	C(18)	1.502(15)
C(14)	C(15)	1.457(12)	C(14)	C(19)	1.491(12)
C(15)	C(20)	1.506(12)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(6)	H(1)	0.950	C(6)	H(2)	0.950
C(6)	H(3)	0.950	C(7)	H(4)	0.950
C(7)	H(5)	0.950	C(7)	H(6)	0.950
C(8)	H(7)	0.950	C(8)	H(8)	0.950
C(8)	H(9)	0.950	C(9)	H(10)	0.950
C(9)	H(11)	0.950	C(9)	H(12)	0.950
C(10)	H(13)	0.950	C(10)	H(14)	0.950
C(10)	H(15)	0.950	C(16)	H(16)	0.950
C(16)	H(17)	0.950	C(16)	H(18)	0.950
C(17)	H(19)	0.950	C(17)	H(20)	0.950
C(17)	H(21)	0.950	C(18)	H(22)	0.950
C(18)	H(23)	0.950	C(18)	H(24)	0.950
C(19)	H(25)	0.950	C(19)	H(26)	0.950
C(19)	H(27)	0.950	C(20)	H(28)	0.950
C(20)	H(29)	0.950	C(20)	H(30)	0.950
C(21)	H(31)	0.950	C(21)	H(32)	0.950
C(21)	H(33)	0.950	C(22)	H(34)	0.950
C(22)	H(35)	0.950	C(22)	H(36)	0.950
C(23)	H(37)	0.950	C(23)	H(38)	0.950
C(24)	H(39)	0.950	C(24)	H(40)	0.950
C(24)	H(41)	0.950	C(25)	H(42)	0.950
C(25)	H(43)	0.950	C(25)	H(44)	0.950

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Ir(2)	Ir(1)	P(1)	86.75(5)	Ir(2)	Ir(1)	C(1)	132.5(2)
Ir(2)	Ir(1)	C(2)	102.6(2)	Ir(2)	Ir(1)	C(3)	98.8(2)
Ir(2)	Ir(1)	C(4)	127.1(2)	Ir(2)	Ir(1)	C(5)	160.4(2)
P(1)	Ir(1)	C(1)	106.9(2)	P(1)	Ir(1)	C(2)	131.6(2)
P(1)	Ir(1)	C(3)	166.8(2)	P(1)	Ir(1)	C(4)	143.9(2)
P(1)	Ir(1)	C(5)	111.7(2)	C(1)	Ir(1)	C(2)	35.5(3)
C(1)	Ir(1)	C(3)	60.6(3)	C(1)	Ir(1)	C(4)	61.6(3)
C(1)	Ir(1)	C(5)	37.8(3)	C(2)	Ir(1)	C(3)	35.5(3)
C(2)	Ir(1)	C(4)	59.7(3)	C(2)	Ir(1)	C(5)	60.7(3)
C(3)	Ir(1)	C(4)	36.6(3)	C(3)	Ir(1)	C(5)	61.8(3)
C(4)	Ir(1)	C(5)	37.3(3)	Ir(1)	Ir(2)	P(2)	84.94(5)
Ir(1)	Ir(2)	C(11)	129.3(2)	Ir(1)	Ir(2)	C(12)	163.5(2)
Ir(1)	Ir(2)	C(13)	134.3(2)	Ir(1)	Ir(2)	C(14)	104.53(19)
Ir(1)	Ir(2)	C(15)	101.65(19)	P(2)	Ir(2)	C(11)	143.49(19)
P(2)	Ir(2)	C(12)	110.6(2)	P(2)	Ir(2)	C(13)	105.5(2)
P(2)	Ir(2)	C(14)	129.4(2)	P(2)	Ir(2)	C(15)	166.0(2)
C(11)	Ir(2)	C(12)	37.7(3)	C(11)	Ir(2)	C(13)	62.1(3)
C(11)	Ir(2)	C(14)	61.3(2)	C(11)	Ir(2)	C(15)	36.3(2)
C(12)	Ir(2)	C(13)	38.0(3)	C(12)	Ir(2)	C(14)	61.7(2)
C(12)	Ir(2)	C(15)	62.0(2)	C(13)	Ir(2)	C(14)	35.5(2)
C(13)	Ir(2)	C(15)	61.1(3)	C(14)	Ir(2)	C(15)	37.1(3)
Ir(1)	P(1)	C(21)	118.3(3)	Ir(1)	P(1)	C(22)	117.6(4)
Ir(1)	P(1)	C(23)	116.4(3)	C(21)	P(1)	C(22)	98.0(5)
C(21)	P(1)	C(23)	100.6(5)	C(22)	P(1)	C(23)	102.8(6)
Ir(2)	P(2)	C(23)	115.4(3)	Ir(2)	P(2)	C(24)	118.5(3)
Ir(2)	P(2)	C(25)	117.6(3)	C(23)	P(2)	C(24)	100.0(5)
C(23)	P(2)	C(25)	100.2(6)	C(24)	P(2)	C(25)	102.1(5)
Ir(1)	C(1)	C(2)	73.0(5)	Ir(1)	C(1)	C(5)	69.3(5)
Ir(1)	C(1)	C(6)	130.1(7)	C(2)	C(1)	C(5)	106.5(8)
C(2)	C(1)	C(6)	128.0(9)	C(5)	C(1)	C(6)	124.8(9)

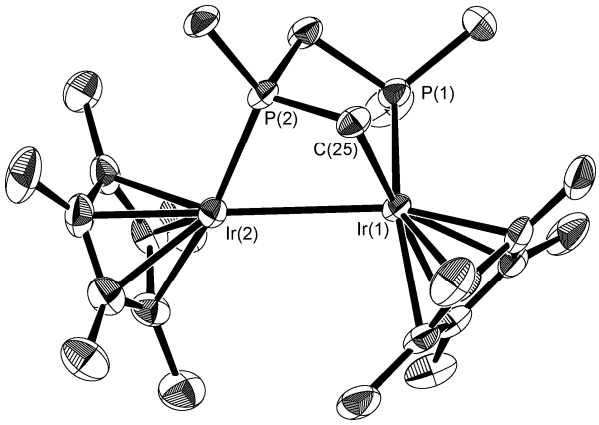
Ir(1)	C(2)	C(1)	71.5(5)	Ir(1)	C(2)	C(3)	70.6(5)
Ir(1)	C(2)	C(7)	130.9(6)	C(1)	C(2)	C(3)	110.7(7)
C(1)	C(2)	C(7)	125.4(9)	C(3)	C(2)	C(7)	123.4(9)
Ir(1)	C(3)	C(2)	73.9(5)	Ir(1)	C(3)	C(4)	70.6(5)
Ir(1)	C(3)	C(8)	127.6(6)	C(2)	C(3)	C(4)	107.6(8)
C(2)	C(3)	C(8)	125.3(8)	C(4)	C(3)	C(8)	126.5(9)
Ir(1)	C(4)	C(3)	72.8(5)	Ir(1)	C(4)	C(5)	71.4(5)
Ir(1)	C(4)	C(9)	124.4(7)	C(3)	C(4)	C(5)	108.8(8)
C(3)	C(4)	C(9)	127.8(10)	C(5)	C(4)	C(9)	123.3(10)
Ir(1)	C(5)	C(1)	73.0(5)	Ir(1)	C(5)	C(4)	71.3(5)
Ir(1)	C(5)	C(10)	128.1(8)	C(1)	C(5)	C(4)	106.3(8)
C(1)	C(5)	C(10)	124.6(10)	C(4)	C(5)	C(10)	128.4(10)
Ir(2)	C(11)	C(12)	71.0(4)	Ir(2)	C(11)	C(15)	72.7(4)
Ir(2)	C(11)	C(16)	124.7(5)	C(12)	C(11)	C(15)	108.8(7)
C(12)	C(11)	C(16)	126.3(7)	C(15)	C(11)	C(16)	124.9(7)
Ir(2)	C(12)	C(11)	71.2(4)	Ir(2)	C(12)	C(13)	72.4(4)
Ir(2)	C(12)	C(17)	128.3(6)	C(11)	C(12)	C(13)	106.0(6)
C(11)	C(12)	C(17)	126.6(8)	C(13)	C(12)	C(17)	126.8(8)
Ir(2)	C(13)	C(12)	69.6(4)	Ir(2)	C(13)	C(14)	73.6(5)
Ir(2)	C(13)	C(18)	131.0(7)	C(12)	C(13)	C(14)	108.9(7)
C(12)	C(13)	C(18)	123.0(8)	C(14)	C(13)	C(18)	127.2(8)
Ir(2)	C(14)	C(13)	70.9(4)	Ir(2)	C(14)	C(15)	69.7(4)
Ir(2)	C(14)	C(19)	132.1(5)	C(13)	C(14)	C(15)	107.8(7)
C(13)	C(14)	C(19)	126.9(8)	C(15)	C(14)	C(19)	124.6(7)
Ir(2)	C(15)	C(11)	71.0(4)	Ir(2)	C(15)	C(14)	73.2(4)
Ir(2)	C(15)	C(20)	130.2(5)	C(11)	C(15)	C(14)	108.5(7)
C(11)	C(15)	C(20)	129.3(8)	C(14)	C(15)	C(20)	121.3(7)
P(1)	C(23)	P(2)	105.3(6)				

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(6)	H(1)	110.2	C(1)	C(6)	H(2)	109.5
C(1)	C(6)	H(3)	108.8	H(1)	C(6)	H(2)	109.5
H(1)	C(6)	H(3)	109.5	H(2)	C(6)	H(3)	109.5
C(2)	C(7)	H(4)	110.4	C(2)	C(7)	H(5)	108.4
C(2)	C(7)	H(6)	109.6	H(4)	C(7)	H(5)	109.5
H(4)	C(7)	H(6)	109.5	H(5)	C(7)	H(6)	109.5
C(3)	C(8)	H(7)	109.7	C(3)	C(8)	H(8)	109.2
C(3)	C(8)	H(9)	109.5	H(7)	C(8)	H(8)	109.5
H(7)	C(8)	H(9)	109.5	H(8)	C(8)	H(9)	109.5
C(4)	C(9)	H(10)	109.8	C(4)	C(9)	H(11)	109.4
C(4)	C(9)	H(12)	109.2	H(10)	C(9)	H(11)	109.5
H(10)	C(9)	H(12)	109.5	H(11)	C(9)	H(12)	109.5
C(5)	C(10)	H(13)	109.8	C(5)	C(10)	H(14)	109.5
C(5)	C(10)	H(15)	109.1	H(13)	C(10)	H(14)	109.5
H(13)	C(10)	H(15)	109.5	H(14)	C(10)	H(15)	109.5
C(11)	C(16)	H(16)	109.8	C(11)	C(16)	H(17)	109.2
C(11)	C(16)	H(18)	109.4	H(16)	C(16)	H(17)	109.5
H(16)	C(16)	H(18)	109.5	H(17)	C(16)	H(18)	109.5
C(12)	C(17)	H(19)	110.2	C(12)	C(17)	H(20)	109.3
C(12)	C(17)	H(21)	108.8	H(19)	C(17)	H(20)	109.5
H(19)	C(17)	H(21)	109.5	H(20)	C(17)	H(21)	109.5
C(13)	C(18)	H(22)	108.6	C(13)	C(18)	H(23)	109.8
C(13)	C(18)	H(24)	110.0	H(22)	C(18)	H(23)	109.5
H(22)	C(18)	H(24)	109.5	H(23)	C(18)	H(24)	109.5
C(14)	C(19)	H(25)	109.2	C(14)	C(19)	H(26)	109.6
C(14)	C(19)	H(27)	109.6	H(25)	C(19)	H(26)	109.5
H(25)	C(19)	H(27)	109.5	H(26)	C(19)	H(27)	109.5
C(15)	C(20)	H(28)	109.4	C(15)	C(20)	H(29)	109.5
C(15)	C(20)	H(30)	109.5	H(28)	C(20)	H(29)	109.5
H(28)	C(20)	H(30)	109.5	H(29)	C(20)	H(30)	109.5

P(1)	C(21)	H(31)	110.0	P(1)	C(21)	H(32)	109.1
P(1)	C(21)	H(33)	109.3	H(31)	C(21)	H(32)	109.5
H(31)	C(21)	H(33)	109.5	H(32)	C(21)	H(33)	109.5
P(1)	C(22)	H(34)	109.3	P(1)	C(22)	H(35)	109.5
P(1)	C(22)	H(36)	109.6	H(34)	C(22)	H(35)	109.5
H(34)	C(22)	H(36)	109.5	H(35)	C(22)	H(36)	109.5
P(1)	C(23)	H(37)	109.9	P(1)	C(23)	H(38)	111.3
P(2)	C(23)	H(37)	109.8	P(2)	C(23)	H(38)	111.0
H(37)	C(23)	H(38)	109.5	P(2)	C(24)	H(39)	109.6
P(2)	C(24)	H(40)	109.9	P(2)	C(24)	H(41)	108.8
H(39)	C(24)	H(40)	109.5	H(39)	C(24)	H(41)	109.5
H(40)	C(24)	H(41)	109.5	P(2)	C(25)	H(42)	109.8
P(2)	C(25)	H(43)	109.1	P(2)	C(25)	H(44)	109.6
H(42)	C(25)	H(43)	109.5	H(42)	C(25)	H(44)	109.5
H(43)	C(25)	H(44)	109.5				

Details of the X-ray crystal structures for complex 8



A. Crystal Data

Empirical Formula	$C_{26}H_{45}F_3O_3P_2SIr_2$
Formula Weight	941.08
Crystal Color, Habit	orange, block
Crystal Dimensions	0.60 X 0.30 X 0.30 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2θ range)	25 (29.4 - 29.9^o)
Omega Scan Peak Width	
at Half-height	0.18^o
Lattice Parameters	a = 9.771(3) Å
	b = 10.880(3) Å
	c = 15.431(3) Å
	α = 80.236(19) ^{o}
	β = 83.09(2) ^{o}
	γ = 86.91(3) ^{o}
	V = 1604.0(8) Å^3
Space Group	P-1 (#2)

Z value	2
D_{calc}	1.948 g/cm^3
F_{000}	904.00
μ(MoKα)	85.182 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5S
Radiation	MoKα (λ = 0.71069 Å)
	graphite monochromated
Attenuator	Zr foil (factors = 1.00, 2.25, 5.26, 11.83)
Take-off Angle	6.0^o
Detector Aperture	13.0 mm horizontal
	9.0 mm vertical
Crystal to Detector Distance	258 mm
Voltage, Current	50 kV, 20 mA
Temperature	23.0^{o}C
Scan Type	ω-2θ
Scan Rate	2.0^o/min (in ω)
Scan Width	(1.31 + 0.30 tan θ)^o
$2\theta_{max}$	55.0^o
No. of Reflections Measured	Total: 7637
	Unique: 7354 (R_{int} = 0.020)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.063 - 0.078)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF99 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1/[0.0016Fo^2+1.0000σ(Fo^2)]
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms

No. Observations (I>3.00σ(I))	5063
No. Variables	377
Reflection/Parameter Ratio	13.43
Residuals: R (I>3.00σ(I))	0.0375
Residuals: Rw (I>3.00σ(I))	0.0497
Goodness of Fit Indicator	1.019
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	2.36 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.70 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ir(1)	0.66137(3)	0.16787(3)	0.16242(2)	2.976(6)
Ir(2)	0.58550(3)	0.23142(3)	0.34551(2)	3.147(7)
S(1)	1.0143(3)	0.3123(3)	0.7784(2)	6.85(8)
P(1)	0.8314(2)	0.3061(2)	0.13932(15)	3.82(4)
P(2)	0.8071(2)	0.1731(2)	0.31764(14)	3.35(4)
F(1)	0.9396(14)	0.3708(12)	0.6215(7)	14.3(4)
F(2)	0.9869(14)	0.1799(11)	0.6582(7)	15.1(4)
F(3)	0.7975(10)	0.2631(13)	0.7123(8)	13.4(4)
O(1)	0.9374(13)	0.4179(9)	0.8055(9)	10.9(3)
O(2)	1.1507(11)	0.3339(15)	0.7385(9)	14.6(5)
O(3)	0.9993(10)	0.1986(9)	0.8414(6)	8.9(2)
C(1)	0.5778(10)	-0.0034(8)	0.1274(6)	4.3(2)
C(2)	0.4638(9)	0.0801(9)	0.1453(6)	4.4(2)
C(3)	0.4844(10)	0.1934(9)	0.0828(6)	4.6(2)
C(4)	0.6055(9)	0.1818(9)	0.0262(5)	4.4(2)
C(5)	0.6705(10)	0.0573(9)	0.0559(5)	4.5(2)
C(6)	0.5987(15)	-0.1324(9)	0.1742(8)	6.9(3)
C(7)	0.3422(11)	0.0513(12)	0.2154(7)	7.2(3)
C(8)	0.3814(12)	0.3010(10)	0.0735(9)	6.8(3)
C(9)	0.6570(14)	0.2699(12)	-0.0536(7)	7.3(3)
C(10)	0.7940(12)	-0.0028(11)	0.0113(7)	6.6(3)
C(11)	0.5919(10)	0.3870(9)	0.4246(6)	4.9(2)
C(12)	0.5328(12)	0.2716(9)	0.4792(6)	5.3(2)
C(13)	0.4099(11)	0.2503(9)	0.4477(7)	5.1(2)
C(14)	0.3880(9)	0.3403(9)	0.3742(7)	4.8(2)
C(15)	0.5019(11)	0.4268(7)	0.3598(7)	4.7(2)
C(16)	0.7143(12)	0.4530(11)	0.4399(8)	7.4(3)
C(17)	0.5923(17)	0.2015(14)	0.5632(7)	8.6(4)
C(18)	0.3128(12)	0.1487(11)	0.4918(8)	7.3(3)
C(19)	0.2614(11)	0.3579(11)	0.3276(9)	6.9(3)

C(20)	0.5117(15)	0.5439(10)	0.2930(9)	8.0(3)
C(21)	0.9783(11)	0.2757(14)	0.0615(7)	7.2(3)
C(22)	0.7862(13)	0.4667(9)	0.1015(8)	7.0(3)
C(23)	0.9046(9)	0.2967(8)	0.2449(5)	4.3(2)
C(24)	0.9167(9)	0.1210(10)	0.4056(6)	4.7(2)
C(25)	0.8059(8)	0.0654(7)	0.2450(5)	3.80(18)
C(26)	0.9340(16)	0.2763(15)	0.6893(11)	8.3(4)

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.6797	-0.1685	0.1467	8.51
H(2)	0.5216	-0.1803	0.1709	8.51
H(3)	0.6091	-0.1311	0.2344	8.51
H(4)	0.3542	-0.0306	0.2472	8.65
H(5)	0.2601	0.0565	0.1875	8.65
H(6)	0.3357	0.1098	0.2551	8.65
H(7)	0.3059	0.2864	0.1184	8.39
H(8)	0.3488	0.3104	0.0171	8.40
H(9)	0.4251	0.3748	0.0788	8.40
H(10)	0.5970	0.3418	-0.0584	8.70
H(11)	0.6587	0.2324	-0.1050	8.71
H(12)	0.7474	0.2934	-0.0480	8.71
H(13)	0.8321	0.0542	-0.0383	8.40
H(14)	0.7675	-0.0755	-0.0081	8.40
H(15)	0.8610	-0.0251	0.0515	8.40
H(16)	0.7523	0.4109	0.4912	9.50
H(17)	0.6873	0.5360	0.4476	9.50
H(18)	0.7815	0.4547	0.3899	9.50
H(19)	0.5362	0.1334	0.5896	10.45
H(20)	0.5934	0.2579	0.6039	10.45
H(21)	0.6836	0.1714	0.5481	10.45
H(22)	0.2362	0.1509	0.4590	8.42
H(23)	0.2815	0.1629	0.5501	8.42
H(24)	0.3590	0.0692	0.4945	8.42
H(25)	0.2698	0.4298	0.2831	8.37
H(26)	0.1841	0.3691	0.3695	8.37
H(27)	0.2491	0.2870	0.3013	8.37
H(28)	0.5938	0.5865	0.2937	9.11
H(29)	0.4339	0.5970	0.3053	9.11
H(30)	0.5100	0.5212	0.2364	9.12

H(31)	1.0456	0.2252	0.0919	8.80
H(32)	1.0171	0.3526	0.0335	8.80
H(33)	0.9492	0.2337	0.0181	8.79
H(34)	0.7956	0.4826	0.0386	8.39
H(35)	0.8456	0.5187	0.1224	8.39
H(36)	0.6934	0.4838	0.1236	8.39
H(37)	1.0002	0.2744	0.2385	5.21
H(38)	0.8914	0.3734	0.2669	5.21
H(39)	0.9602	0.1910	0.4181	5.73
H(40)	0.9851	0.0626	0.3869	5.73
H(41)	0.8623	0.0828	0.4573	5.74
H(42)	0.7724	-0.0129	0.2743	4.64
H(43)	0.8938	0.0534	0.2133	4.64

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03934(17)	0.03957(18)	0.03522(18)	-0.00645(13)	-0.01188(13)	-0.00218(13)
Ir(2)	0.04570(19)	0.03565(17)	0.03875(19)	-0.00601(13)	-0.00656(14)	-0.00487(13)
S(1)	0.087(2)	0.084(2)	0.086(2)	-0.0167(17)	-0.0237(17)	0.0092(17)
P(1)	0.0491(12)	0.0563(13)	0.0395(11)	-0.0185(10)	-0.0097(9)	0.0014(9)
P(2)	0.0458(11)	0.0443(11)	0.0398(11)	-0.0055(9)	-0.0177(9)	-0.0042(8)
F(1)	0.257(14)	0.182(10)	0.095(7)	0.049(10)	-0.068(8)	0.019(7)
F(2)	0.274(15)	0.176(10)	0.148(10)	0.117(10)	-0.079(9)	-0.091(8)
F(3)	0.088(6)	0.238(13)	0.195(12)	-0.026(7)	-0.047(6)	-0.042(10)
O(1)	0.172(11)	0.074(6)	0.191(12)	0.009(6)	-0.085(9)	-0.040(7)
O(2)	0.082(7)	0.241(15)	0.212(15)	-0.072(8)	-0.017(8)	0.043(11)
O(3)	0.127(8)	0.105(7)	0.084(6)	0.022(6)	-0.003(5)	0.030(5)
C(1)	0.072(6)	0.043(4)	0.053(5)	-0.014(4)	-0.030(4)	-0.006(4)
C(2)	0.056(5)	0.059(5)	0.057(5)	-0.022(4)	-0.023(4)	-0.005(4)
C(3)	0.061(5)	0.060(5)	0.062(6)	-0.002(4)	-0.037(4)	-0.011(4)
C(4)	0.055(5)	0.077(6)	0.039(4)	-0.017(4)	-0.015(3)	-0.011(4)
C(5)	0.072(6)	0.065(5)	0.039(4)	-0.010(4)	-0.019(4)	-0.015(4)
C(6)	0.132(11)	0.048(5)	0.090(8)	-0.017(6)	-0.041(8)	-0.008(5)
C(7)	0.076(7)	0.126(11)	0.071(7)	-0.061(7)	-0.015(6)	0.001(7)
C(8)	0.073(7)	0.074(7)	0.119(11)	-0.006(6)	-0.048(7)	-0.006(7)
C(9)	0.113(9)	0.112(10)	0.051(6)	-0.047(8)	-0.042(6)	0.024(6)
C(10)	0.097(8)	0.101(9)	0.067(7)	0.002(7)	-0.020(6)	-0.049(7)
C(11)	0.073(6)	0.056(5)	0.059(6)	-0.014(4)	0.014(5)	-0.028(4)
C(12)	0.093(7)	0.062(6)	0.051(5)	-0.018(5)	0.005(5)	-0.025(4)
C(13)	0.069(6)	0.047(5)	0.074(7)	-0.012(4)	0.010(5)	-0.013(4)
C(14)	0.049(5)	0.052(5)	0.080(7)	0.006(4)	-0.003(4)	-0.016(5)
C(15)	0.079(6)	0.029(4)	0.066(6)	0.004(4)	0.007(5)	-0.005(4)
C(16)	0.090(8)	0.100(9)	0.111(10)	-0.025(7)	-0.006(7)	-0.073(8)
C(17)	0.162(14)	0.124(12)	0.044(6)	-0.020(10)	-0.026(7)	-0.005(7)
C(18)	0.083(8)	0.079(8)	0.104(10)	-0.022(6)	0.018(7)	0.003(7)
C(19)	0.068(7)	0.080(8)	0.117(11)	0.022(6)	-0.020(7)	-0.029(7)

C(20)	0.133(12)	0.045(6)	0.111(10)	0.011(6)	0.024(9)	-0.000(6)
C(21)	0.060(6)	0.158(13)	0.060(7)	-0.038(7)	0.015(5)	-0.033(7)
C(22)	0.112(10)	0.064(6)	0.090(8)	-0.037(6)	-0.046(7)	0.020(6)
C(23)	0.058(5)	0.056(5)	0.051(5)	-0.020(4)	-0.016(4)	-0.005(4)
C(24)	0.056(5)	0.079(6)	0.047(5)	-0.008(4)	-0.026(4)	0.001(4)
C(25)	0.048(4)	0.046(4)	0.053(5)	0.006(3)	-0.021(3)	-0.006(3)
C(26)	0.094(10)	0.094(10)	0.123(13)	0.021(8)	-0.024(9)	-0.001(9)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ir(1)	Ir(2)	3.0188(4)	Ir(1)	P(1)	2.257(2)
Ir(1)	C(1)	2.245(9)	Ir(1)	C(2)	2.261(10)
Ir(1)	C(3)	2.218(10)	Ir(1)	C(4)	2.213(9)
Ir(1)	C(5)	2.186(10)	Ir(1)	C(25)	2.155(8)
Ir(2)	P(2)	2.235(2)	Ir(2)	C(11)	2.256(11)
Ir(2)	C(12)	2.177(10)	Ir(2)	C(13)	2.212(10)
Ir(2)	C(14)	2.247(9)	Ir(2)	C(15)	2.272(8)
S(1)	O(1)	1.433(12)	S(1)	O(2)	1.414(11)
S(1)	O(3)	1.440(9)	S(1)	C(26)	1.770(19)
P(1)	C(21)	1.812(11)	P(1)	C(22)	1.795(10)
P(1)	C(23)	1.842(9)	P(2)	C(23)	1.829(8)
P(2)	C(24)	1.826(10)	P(2)	C(25)	1.755(9)
F(1)	C(26)	1.334(19)	F(2)	C(26)	1.28(2)
F(3)	C(26)	1.347(18)	C(1)	C(2)	1.430(13)
C(1)	C(5)	1.431(12)	C(1)	C(6)	1.481(13)
C(2)	C(3)	1.438(12)	C(2)	C(7)	1.515(13)
C(3)	C(4)	1.397(12)	C(3)	C(8)	1.501(14)
C(4)	C(5)	1.488(13)	C(4)	C(9)	1.480(14)
C(5)	C(10)	1.492(15)	C(11)	C(12)	1.491(13)
C(11)	C(15)	1.410(15)	C(11)	C(16)	1.490(17)
C(12)	C(13)	1.393(16)	C(12)	C(17)	1.548(17)
C(13)	C(14)	1.396(14)	C(13)	C(18)	1.513(15)
C(14)	C(15)	1.468(14)	C(14)	C(19)	1.492(16)
C(15)	C(20)	1.496(14)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(6)	H(1)	0.950	C(6)	H(2)	0.950
C(6)	H(3)	0.950	C(7)	H(4)	0.950
C(7)	H(5)	0.950	C(7)	H(6)	0.950
C(8)	H(7)	0.950	C(8)	H(8)	0.950
C(8)	H(9)	0.950	C(9)	H(10)	0.950
C(9)	H(11)	0.950	C(9)	H(12)	0.950
C(10)	H(13)	0.950	C(10)	H(14)	0.950
C(10)	H(15)	0.950	C(16)	H(16)	0.950
C(16)	H(17)	0.950	C(16)	H(18)	0.950
C(17)	H(19)	0.950	C(17)	H(20)	0.950
C(17)	H(21)	0.950	C(18)	H(22)	0.950
C(18)	H(23)	0.950	C(18)	H(24)	0.950
C(19)	H(25)	0.950	C(19)	H(26)	0.950
C(19)	H(27)	0.950	C(20)	H(28)	0.950
C(20)	H(29)	0.950	C(20)	H(30)	0.950
C(21)	H(31)	0.950	C(21)	H(32)	0.950
C(21)	H(33)	0.950	C(22)	H(34)	0.950
C(22)	H(35)	0.950	C(22)	H(36)	0.950
C(23)	H(37)	0.950	C(23)	H(38)	0.950
C(24)	H(39)	0.950	C(24)	H(40)	0.950
C(24)	H(41)	0.950	C(25)	H(42)	0.950
C(25)	H(43)	0.950			

Table 6. Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
Ir(2)	Ir(1)	P(1)	89.34(6)	Ir(2)	Ir(1)	C(1)	119.6(2)
Ir(2)	Ir(1)	C(2)	99.5(2)	Ir(2)	Ir(1)	C(3)	112.5(2)
Ir(2)	Ir(1)	C(4)	147.4(2)	Ir(2)	Ir(1)	C(5)	157.2(2)
Ir(2)	Ir(1)	C(25)	73.4(2)	P(1)	Ir(1)	C(1)	148.0(2)
P(1)	Ir(1)	C(2)	159.2(2)	P(1)	Ir(1)	C(3)	121.7(2)
P(1)	Ir(1)	C(4)	100.4(2)	P(1)	Ir(1)	C(5)	112.1(2)
P(1)	Ir(1)	C(25)	80.3(2)	C(1)	Ir(1)	C(2)	37.0(3)
C(1)	Ir(1)	C(3)	62.3(3)	C(1)	Ir(1)	C(4)	63.2(3)
C(1)	Ir(1)	C(5)	37.7(3)	C(1)	Ir(1)	C(25)	94.5(3)
C(2)	Ir(1)	C(3)	37.4(3)	C(2)	Ir(1)	C(4)	62.5(3)
C(2)	Ir(1)	C(5)	63.2(3)	C(2)	Ir(1)	C(25)	120.2(3)
C(3)	Ir(1)	C(4)	36.8(3)	C(3)	Ir(1)	C(5)	63.7(3)
C(3)	Ir(1)	C(25)	156.2(3)	C(4)	Ir(1)	C(5)	39.5(3)
C(4)	Ir(1)	C(25)	138.7(3)	C(5)	Ir(1)	C(25)	101.5(3)
Ir(1)	Ir(2)	P(2)	66.11(5)	Ir(1)	Ir(2)	C(11)	142.1(2)
Ir(1)	Ir(2)	C(12)	178.3(2)	Ir(1)	Ir(2)	C(13)	143.3(3)
Ir(1)	Ir(2)	C(14)	119.2(3)	Ir(1)	Ir(2)	C(15)	119.0(2)
P(2)	Ir(2)	C(11)	103.8(2)	P(2)	Ir(2)	C(12)	113.0(3)
P(2)	Ir(2)	C(13)	146.6(2)	P(2)	Ir(2)	C(14)	164.3(2)
P(2)	Ir(2)	C(15)	126.4(2)	C(11)	Ir(2)	C(12)	39.3(3)
C(11)	Ir(2)	C(13)	63.0(3)	C(11)	Ir(2)	C(14)	62.5(3)
C(11)	Ir(2)	C(15)	36.3(3)	C(12)	Ir(2)	C(13)	37.0(4)
C(12)	Ir(2)	C(14)	62.1(4)	C(12)	Ir(2)	C(15)	62.7(3)
C(13)	Ir(2)	C(14)	36.5(3)	C(13)	Ir(2)	C(15)	62.1(3)
C(14)	Ir(2)	C(15)	37.9(3)	O(1)	S(1)	O(2)	116.2(8)
O(1)	S(1)	O(3)	114.6(6)	O(1)	S(1)	C(26)	105.5(8)
O(2)	S(1)	O(3)	114.4(7)	O(2)	S(1)	C(26)	101.6(8)
O(3)	S(1)	C(26)	101.9(7)	Ir(1)	P(1)	C(21)	116.3(5)
Ir(1)	P(1)	C(22)	117.5(4)	Ir(1)	P(1)	C(23)	107.1(2)
C(21)	P(1)	C(22)	102.9(6)	C(21)	P(1)	C(23)	104.0(4)

C(22)	P(1)	C(23)	108.0(5)	Ir(2)	P(2)	C(23)	111.5(2)
Ir(2)	P(2)	C(24)	122.4(3)	Ir(2)	P(2)	C(25)	104.5(3)
C(23)	P(2)	C(24)	103.6(4)	C(23)	P(2)	C(25)	99.8(4)
C(24)	P(2)	C(25)	112.8(4)	Ir(1)	C(1)	C(2)	72.1(5)
Ir(1)	C(1)	C(5)	68.9(5)	Ir(1)	C(1)	C(6)	125.2(8)
C(2)	C(1)	C(5)	109.1(7)	C(2)	C(1)	C(6)	126.2(8)
C(5)	C(1)	C(6)	124.6(9)	Ir(1)	C(2)	C(1)	70.9(5)
Ir(1)	C(2)	C(3)	69.7(5)	Ir(1)	C(2)	C(7)	126.3(7)
C(1)	C(2)	C(3)	107.3(7)	C(1)	C(2)	C(7)	125.8(8)
C(3)	C(2)	C(7)	126.9(9)	Ir(1)	C(3)	C(2)	72.9(5)
Ir(1)	C(3)	C(4)	71.4(5)	Ir(1)	C(3)	C(8)	127.9(8)
C(2)	C(3)	C(4)	109.8(8)	C(2)	C(3)	C(8)	124.3(8)
C(4)	C(3)	C(8)	125.5(8)	Ir(1)	C(4)	C(3)	71.8(5)
Ir(1)	C(4)	C(5)	69.3(5)	Ir(1)	C(4)	C(9)	128.0(8)
C(3)	C(4)	C(5)	107.4(7)	C(3)	C(4)	C(9)	127.6(9)
C(5)	C(4)	C(9)	124.8(8)	Ir(1)	C(5)	C(1)	73.4(5)
Ir(1)	C(5)	C(4)	71.2(5)	Ir(1)	C(5)	C(10)	128.3(8)
C(1)	C(5)	C(4)	106.3(7)	C(1)	C(5)	C(10)	125.6(8)
C(4)	C(5)	C(10)	127.3(8)	Ir(2)	C(11)	C(12)	67.5(5)
Ir(2)	C(11)	C(15)	72.5(6)	Ir(2)	C(11)	C(16)	128.3(7)
C(12)	C(11)	C(15)	105.9(9)	C(12)	C(11)	C(16)	127.1(9)
C(15)	C(11)	C(16)	126.8(9)	Ir(2)	C(12)	C(11)	73.2(5)
Ir(2)	C(12)	C(13)	72.9(6)	Ir(2)	C(12)	C(17)	125.8(8)
C(11)	C(12)	C(13)	108.1(8)	C(11)	C(12)	C(17)	123.7(11)
C(13)	C(12)	C(17)	127.7(10)	Ir(2)	C(13)	C(12)	70.1(6)
Ir(2)	C(13)	C(14)	73.1(5)	Ir(2)	C(13)	C(18)	126.1(7)
C(12)	C(13)	C(14)	109.9(8)	C(12)	C(13)	C(18)	123.7(9)
C(14)	C(13)	C(18)	126.3(10)	Ir(2)	C(14)	C(13)	70.4(5)
Ir(2)	C(14)	C(15)	71.9(5)	Ir(2)	C(14)	C(19)	130.3(8)
C(13)	C(14)	C(15)	107.6(9)	C(13)	C(14)	C(19)	126.3(9)
C(15)	C(14)	C(19)	125.5(8)	Ir(2)	C(15)	C(11)	71.2(5)
Ir(2)	C(15)	C(14)	70.1(5)	Ir(2)	C(15)	C(20)	129.0(7)
C(11)	C(15)	C(14)	108.4(8)	C(11)	C(15)	C(20)	126.2(10)

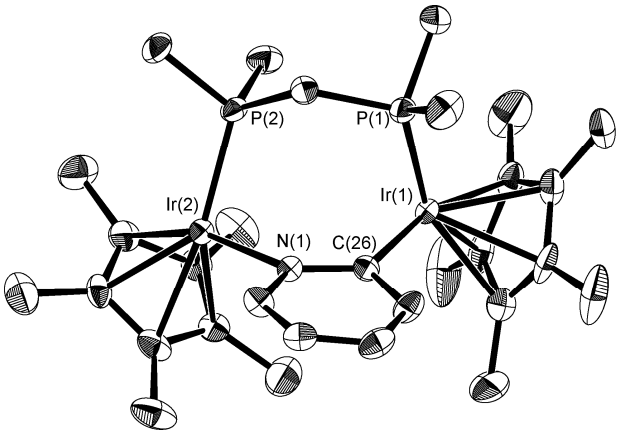
C(14)	C(15)	C(20)	125.1(10)	P(1)	C(23)	P(2)	103.0(4)
Ir(1)	C(25)	P(2)	97.0(3)	S(1)	C(26)	F(1)	111.5(12)
S(1)	C(26)	F(2)	114.2(12)	S(1)	C(26)	F(3)	110.8(12)
F(1)	C(26)	F(2)	106.6(14)	F(1)	C(26)	F(3)	103.2(13)
F(2)	C(26)	F(3)	109.9(15)				

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(6)	H(1)	108.8	C(1)	C(6)	H(2)	109.7
C(1)	C(6)	H(3)	109.9	H(1)	C(6)	H(2)	109.5
H(1)	C(6)	H(3)	109.5	H(2)	C(6)	H(3)	109.5
C(2)	C(7)	H(4)	109.5	C(2)	C(7)	H(5)	109.1
C(2)	C(7)	H(6)	109.8	H(4)	C(7)	H(5)	109.5
H(4)	C(7)	H(6)	109.5	H(5)	C(7)	H(6)	109.5
C(3)	C(8)	H(7)	110.1	C(3)	C(8)	H(8)	109.5
C(3)	C(8)	H(9)	108.9	H(7)	C(8)	H(8)	109.5
H(7)	C(8)	H(9)	109.5	H(8)	C(8)	H(9)	109.5
C(4)	C(9)	H(10)	108.4	C(4)	C(9)	H(11)	110.4
C(4)	C(9)	H(12)	109.6	H(10)	C(9)	H(11)	109.5
H(10)	C(9)	H(12)	109.5	H(11)	C(9)	H(12)	109.5
C(5)	C(10)	H(13)	109.3	C(5)	C(10)	H(14)	109.4
C(5)	C(10)	H(15)	109.7	H(13)	C(10)	H(14)	109.5
H(13)	C(10)	H(15)	109.5	H(14)	C(10)	H(15)	109.5
C(11)	C(16)	H(16)	110.2	C(11)	C(16)	H(17)	109.4
C(11)	C(16)	H(18)	108.8	H(16)	C(16)	H(17)	109.5
H(16)	C(16)	H(18)	109.5	H(17)	C(16)	H(18)	109.5
C(12)	C(17)	H(19)	109.9	C(12)	C(17)	H(20)	108.6
C(12)	C(17)	H(21)	109.9	H(19)	C(17)	H(20)	109.5
H(19)	C(17)	H(21)	109.5	H(20)	C(17)	H(21)	109.5
C(13)	C(18)	H(22)	109.4	C(13)	C(18)	H(23)	108.8
C(13)	C(18)	H(24)	110.3	H(22)	C(18)	H(23)	109.5
H(22)	C(18)	H(24)	109.5	H(23)	C(18)	H(24)	109.5
C(14)	C(19)	H(25)	109.3	C(14)	C(19)	H(26)	108.6
C(14)	C(19)	H(27)	110.4	H(25)	C(19)	H(26)	109.5
H(25)	C(19)	H(27)	109.5	H(26)	C(19)	H(27)	109.5
C(15)	C(20)	H(28)	112.2	C(15)	C(20)	H(29)	108.7
C(15)	C(20)	H(30)	107.5	H(28)	C(20)	H(29)	109.5
H(28)	C(20)	H(30)	109.5	H(29)	C(20)	H(30)	109.5

P(1)	C(21)	H(31)	109.7	P(1)	C(21)	H(32)	109.3
P(1)	C(21)	H(33)	109.5	H(31)	C(21)	H(32)	109.5
H(31)	C(21)	H(33)	109.5	H(32)	C(21)	H(33)	109.5
P(1)	C(22)	H(34)	109.7	P(1)	C(22)	H(35)	109.4
P(1)	C(22)	H(36)	109.3	H(34)	C(22)	H(35)	109.5
H(34)	C(22)	H(36)	109.5	H(35)	C(22)	H(36)	109.5
P(1)	C(23)	H(37)	111.0	P(1)	C(23)	H(38)	111.4
P(2)	C(23)	H(37)	110.8	P(2)	C(23)	H(38)	111.1
H(37)	C(23)	H(38)	109.5	P(2)	C(24)	H(39)	109.1
P(2)	C(24)	H(40)	109.6	P(2)	C(24)	H(41)	109.7
H(39)	C(24)	H(40)	109.5	H(39)	C(24)	H(41)	109.5
H(40)	C(24)	H(41)	109.5	Ir(1)	C(25)	H(42)	112.3
Ir(1)	C(25)	H(43)	112.6	P(2)	C(25)	H(42)	112.3
P(2)	C(25)	H(43)	112.8	H(42)	C(25)	H(43)	109.5

Details of the X-ray crystal structures for complex 12



A. Crystal Data

Empirical Formula	$C_{31}H_{50}NP_2Ir_2SO_3F_3$
Formula Weight	1020.18
Crystal Color, Habit	orange, block
Crystal Dimensions	0.40 X 0.35 X 0.35 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2θ range)	24 (28.7 - 29.9^o)
Omega Scan Peak Width	
at Half-height	0.14^o
Lattice Parameters	a = 17.7878(14) Å
	b = 12.3618(17) Å
	c = 18.402(2) Å
	β = 117.595(7) ^{o}
	V = 3586.1(7) Å^3
Space Group	$P2_1/a$ (#14)
Z value	4
D_{calc}	1.889 g/cm^3

F_{000}	1976.00
μ(MoKα)	76.290 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5S
Radiation	MoKα (λ = 0.71069 Å)
	graphite monochromated
Attenuator	Zr foil (factors = 1.00, 2.25, 5.26, 11.83)
Take-off Angle	6.0^o
Detector Aperture	13.0 mm horizontal
	9.0 mm vertical
Crystal to Detector Distance	258 mm
Voltage, Current	50 kV, 20 mA
Temperature	20.0^oC
Scan Type	ω-2θ
Scan Rate	2.0^o/min (in ω)
Scan Width	$(1.15 + 0.30 \tan \theta)^o$
$2\theta_{max}$	55.0^o
No. of Reflections Measured	Total: 8475
	Unique: 8206 (R_{int} = 0.023)
Corrections	Lorentz-polarization
	Absorption
	(trans. factors: 0.042 - 0.069)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF99 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	$\Sigma w (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$1/[0.0025Fo^2+1.0000\sigma(Fo^2)]$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	5785
No. Variables	436

Reflection/Parameter Ratio	13.27
Residuals: R (I>3.00σ(I))	0.0426
Residuals: Rw (I>3.00σ(I))	0.0598
Goodness of Fit Indicator	1.007
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	5.55 $e^-/Å^3$
Minimum peak in Final Diff. Map	-2.43 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ir(1)	0.67122(2)	0.24886(3)	0.32230(2)	2.573(7)
Ir(2)	0.56875(2)	0.29872(3)	0.07868(2)	2.572(7)
S(1)	0.3331(2)	0.7506(3)	0.2553(2)	5.82(8)
P(1)	0.73176(16)	0.4081(2)	0.32338(15)	3.32(5)
P(2)	0.69718(15)	0.3771(2)	0.14211(15)	2.99(5)
F(1)	0.4925(6)	0.7147(10)	0.2998(7)	10.3(3)
F(2)	0.4468(6)	0.6426(9)	0.3769(5)	10.4(3)
F(3)	0.4695(6)	0.8114(8)	0.3847(6)	9.3(3)
O(1)	0.3445(10)	0.8483(11)	0.2156(7)	12.2(5)
O(2)	0.3153(6)	0.6582(10)	0.2080(6)	9.4(3)
O(3)	0.2894(7)	0.7720(9)	0.3027(7)	7.8(3)
N(1)	0.5301(4)	0.3540(5)	0.1676(4)	2.51(14)
C(1)	0.6968(8)	0.0746(9)	0.3651(6)	4.8(2)
C(2)	0.7695(7)	0.1361(10)	0.4136(6)	4.5(2)
C(3)	0.7475(7)	0.2084(10)	0.4588(6)	4.4(2)
C(4)	0.6601(8)	0.1954(11)	0.4361(6)	5.1(3)
C(5)	0.6269(7)	0.1109(11)	0.3766(6)	4.9(2)
C(6)	0.6986(14)	-0.0272(12)	0.3173(8)	11.0(6)
C(7)	0.8576(8)	0.1116(16)	0.4263(10)	9.6(5)
C(8)	0.8065(9)	0.2822(13)	0.5281(6)	7.3(4)
C(9)	0.6175(12)	0.2479(15)	0.4832(8)	8.8(5)
C(10)	0.5421(9)	0.0628(15)	0.3451(9)	9.7(5)
C(11)	0.4545(6)	0.1980(9)	0.0008(6)	4.3(2)
C(12)	0.4926(7)	0.2326(8)	-0.0454(5)	3.9(2)
C(13)	0.5802(7)	0.1890(9)	-0.0085(6)	4.4(2)
C(14)	0.5895(6)	0.1191(7)	0.0600(5)	3.4(2)
C(15)	0.5152(6)	0.1295(7)	0.0659(6)	3.6(2)
C(16)	0.3662(7)	0.2178(12)	-0.0133(8)	6.3(3)
C(17)	0.4484(9)	0.2917(11)	-0.1268(7)	6.8(3)
C(18)	0.6402(9)	0.1975(12)	-0.0446(8)	6.6(4)

C(19)	0.6648(8)	0.0542(10)	0.1086(7)	6.3(3)
C(20)	0.4955(9)	0.0717(11)	0.1277(7)	6.6(3)
C(21)	0.7053(8)	0.5196(10)	0.3721(7)	6.4(3)
C(22)	0.8468(7)	0.4129(12)	0.3773(6)	6.1(3)
C(23)	0.7079(6)	0.4693(7)	0.2246(5)	3.5(2)
C(24)	0.7922(6)	0.2969(10)	0.1822(7)	4.7(2)
C(25)	0.7189(7)	0.4678(10)	0.0760(6)	5.3(3)
C(26)	0.5603(5)	0.3281(7)	0.2484(5)	2.81(17)
C(27)	0.5122(6)	0.3649(9)	0.2867(6)	4.0(2)
C(28)	0.4395(6)	0.4263(9)	0.2473(7)	4.5(2)
C(29)	0.4162(5)	0.4567(8)	0.1680(6)	3.6(2)
C(30)	0.4592(5)	0.4197(8)	0.1299(5)	3.5(2)
C(31)	0.4403(9)	0.7297(13)	0.3305(10)	6.3(3)

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.7541	-0.0383	0.3235	13.33
H(2)	0.6818	-0.0885	0.3373	13.33
H(3)	0.6601	-0.0169	0.2610	13.33
H(4)	0.8955	0.1609	0.4659	12.10
H(5)	0.8731	0.0396	0.4455	12.10
H(6)	0.8601	0.1205	0.3762	12.11
H(7)	0.7766	0.3214	0.5509	8.15
H(8)	0.8484	0.2382	0.5693	8.15
H(9)	0.8330	0.3314	0.5075	8.15
H(10)	0.5613	0.2205	0.4609	11.48
H(11)	0.6470	0.2311	0.5400	11.48
H(12)	0.6158	0.3241	0.4761	11.48
H(13)	0.5383	0.0040	0.3103	10.90
H(14)	0.5329	0.0374	0.3890	10.90
H(15)	0.5002	0.1153	0.3145	10.90
H(16)	0.3384	0.2618	-0.0608	7.41
H(17)	0.3368	0.1511	-0.0218	7.41
H(18)	0.3666	0.2540	0.0325	7.41
H(19)	0.4867	0.3013	-0.1490	7.42
H(20)	0.3998	0.2533	-0.1649	7.42
H(21)	0.4316	0.3604	-0.1162	7.42
H(22)	0.6907	0.1593	-0.0104	8.79
H(23)	0.6152	0.1671	-0.0981	8.79
H(24)	0.6533	0.2714	-0.0473	8.79
H(25)	0.6576	0.0201	0.1512	7.00
H(26)	0.6715	0.0006	0.0750	7.01
H(27)	0.7138	0.0989	0.1318	7.01
H(28)	0.4395	0.0870	0.1186	8.42
H(29)	0.5015	-0.0040	0.1229	8.41
H(30)	0.5349	0.0949	0.1812	8.41

H(31)	0.7444	0.5223	0.4288	8.69
H(32)	0.7075	0.5857	0.3468	8.69
H(33)	0.6496	0.5091	0.3655	8.69
H(34)	0.8680	0.3959	0.3398	6.88
H(35)	0.8650	0.4834	0.3989	6.88
H(36)	0.8676	0.3618	0.4207	6.88
H(37)	0.7523	0.5187	0.2336	4.02
H(38)	0.6561	0.5077	0.2062	4.02
H(39)	0.8099	0.2873	0.1412	5.84
H(40)	0.8360	0.3313	0.2286	5.85
H(41)	0.7802	0.2283	0.1978	5.85
H(42)	0.7003	0.5388	0.0796	6.57
H(43)	0.7782	0.4687	0.0933	6.58
H(44)	0.6897	0.4434	0.0209	6.58
H(45)	0.5307	0.3463	0.3425	5.38
H(46)	0.4083	0.4495	0.2746	6.12
H(47)	0.3682	0.5019	0.1395	4.33
H(48)	0.4407	0.4392	0.0742	4.06

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	0.03595(19)	0.0332(2)	0.03372(18)	0.00048(15)	0.02045(14)	0.00167(15)
Ir(2)	0.03759(19)	0.02815(18)	0.03469(18)	0.00040(16)	0.01904(14)	-0.00385(15)
S(1)	0.075(2)	0.083(2)	0.0586(18)	0.0338(18)	0.0274(16)	-0.0028(17)
P(1)	0.0476(13)	0.0419(14)	0.0396(12)	-0.0126(11)	0.0227(10)	-0.0059(11)
P(2)	0.0411(12)	0.0347(13)	0.0429(12)	-0.0062(10)	0.0238(10)	0.0002(10)
F(1)	0.078(6)	0.189(12)	0.135(8)	0.009(6)	0.060(6)	-0.033(7)
F(2)	0.141(8)	0.126(8)	0.091(6)	0.049(7)	0.023(6)	0.024(6)
F(3)	0.105(6)	0.116(8)	0.126(8)	-0.025(6)	0.049(6)	-0.048(6)
O(1)	0.254(16)	0.140(11)	0.136(10)	0.113(12)	0.145(11)	0.090(9)
O(2)	0.087(7)	0.130(10)	0.100(7)	0.039(7)	0.009(6)	-0.059(7)
O(3)	0.094(7)	0.106(8)	0.113(8)	0.030(6)	0.061(7)	0.003(6)
N(1)	0.035(3)	0.027(3)	0.036(3)	0.003(3)	0.020(3)	-0.000(3)
C(1)	0.106(9)	0.038(6)	0.047(5)	0.017(6)	0.044(6)	0.013(4)
C(2)	0.057(6)	0.070(8)	0.046(5)	0.024(5)	0.027(5)	0.025(5)
C(3)	0.062(6)	0.067(7)	0.036(5)	0.013(5)	0.022(4)	0.010(4)
C(4)	0.088(8)	0.081(8)	0.048(6)	0.017(7)	0.051(6)	0.024(6)
C(5)	0.063(7)	0.070(8)	0.050(6)	-0.004(6)	0.023(5)	0.010(5)
C(6)	0.28(2)	0.058(9)	0.085(10)	0.059(13)	0.088(13)	0.026(8)
C(7)	0.076(9)	0.18(2)	0.128(13)	0.061(11)	0.062(9)	0.075(13)
C(8)	0.100(11)	0.123(14)	0.035(5)	-0.025(9)	0.015(6)	0.006(6)
C(9)	0.152(16)	0.143(16)	0.068(9)	0.081(13)	0.077(10)	0.047(9)
C(10)	0.103(11)	0.145(17)	0.097(11)	-0.063(11)	0.026(9)	0.053(11)
C(11)	0.049(5)	0.056(6)	0.053(5)	-0.006(5)	0.020(4)	-0.032(5)
C(12)	0.067(6)	0.043(6)	0.033(4)	-0.003(4)	0.020(4)	-0.008(4)
C(13)	0.058(6)	0.062(7)	0.052(5)	-0.014(5)	0.031(5)	-0.027(5)
C(14)	0.057(5)	0.024(4)	0.051(5)	0.004(4)	0.025(4)	-0.011(4)
C(15)	0.061(6)	0.023(4)	0.052(5)	-0.014(4)	0.027(4)	-0.014(4)
C(16)	0.046(6)	0.088(10)	0.101(10)	-0.008(6)	0.031(6)	-0.043(8)
C(17)	0.100(11)	0.075(9)	0.060(7)	-0.004(8)	0.018(7)	0.002(7)
C(18)	0.092(10)	0.096(11)	0.090(10)	-0.029(8)	0.067(8)	-0.041(8)

C(19)	0.083(9)	0.049(7)	0.089(9)	0.012(6)	0.024(7)	-0.024(6)
C(20)	0.118(12)	0.069(9)	0.079(8)	-0.026(8)	0.058(8)	-0.015(7)
C(21)	0.133(12)	0.058(7)	0.083(8)	-0.039(8)	0.077(9)	-0.043(7)
C(22)	0.068(7)	0.098(10)	0.052(6)	-0.039(7)	0.017(5)	0.005(6)
C(23)	0.054(5)	0.030(4)	0.043(4)	-0.009(4)	0.018(4)	0.001(4)
C(24)	0.043(5)	0.070(8)	0.073(7)	-0.001(5)	0.031(5)	-0.003(6)
C(25)	0.088(8)	0.067(8)	0.054(6)	-0.038(6)	0.039(6)	-0.004(5)
C(26)	0.041(4)	0.029(4)	0.036(4)	-0.006(3)	0.017(3)	-0.008(3)
C(27)	0.054(5)	0.056(6)	0.061(6)	0.013(5)	0.043(5)	0.005(5)
C(28)	0.064(6)	0.051(6)	0.079(7)	0.002(5)	0.054(6)	-0.006(5)
C(29)	0.039(4)	0.036(5)	0.062(6)	0.008(4)	0.025(4)	0.000(4)
C(30)	0.040(4)	0.041(5)	0.047(5)	0.010(4)	0.017(4)	-0.005(4)
C(31)	0.075(8)	0.073(10)	0.087(10)	-0.000(7)	0.033(8)	-0.020(8)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ir(1)	P(1)	2.240(2)	Ir(1)	C(1)	2.266(11)
Ir(1)	C(2)	2.259(10)	Ir(1)	C(3)	2.290(9)
Ir(1)	C(4)	2.290(14)	Ir(1)	C(5)	2.293(14)
Ir(1)	C(26)	2.054(8)	Ir(2)	P(2)	2.247(2)
Ir(2)	N(1)	2.159(8)	Ir(2)	C(11)	2.245(10)
Ir(2)	C(12)	2.203(8)	Ir(2)	C(13)	2.182(13)
Ir(2)	C(14)	2.303(9)	Ir(2)	C(15)	2.265(9)
S(1)	O(1)	1.473(16)	S(1)	O(2)	1.381(12)
S(1)	O(3)	1.435(16)	S(1)	C(31)	1.782(14)
P(1)	C(21)	1.820(14)	P(1)	C(22)	1.815(11)
P(1)	C(23)	1.828(10)	P(2)	C(23)	1.836(10)
P(2)	C(24)	1.797(11)	P(2)	C(25)	1.822(14)
F(1)	C(31)	1.31(2)	F(2)	C(31)	1.35(2)
F(3)	C(31)	1.344(19)	N(1)	C(26)	1.364(11)
N(1)	C(30)	1.385(11)	C(1)	C(2)	1.406(15)
C(1)	C(5)	1.43(2)	C(1)	C(6)	1.54(2)
C(2)	C(3)	1.395(19)	C(2)	C(7)	1.50(2)
C(3)	C(4)	1.419(19)	C(3)	C(8)	1.523(16)
C(4)	C(5)	1.428(17)	C(4)	C(9)	1.53(2)
C(5)	C(10)	1.47(2)	C(11)	C(12)	1.379(19)
C(11)	C(15)	1.456(13)	C(11)	C(16)	1.488(18)
C(12)	C(13)	1.483(16)	C(12)	C(17)	1.519(15)
C(13)	C(14)	1.475(16)	C(13)	C(18)	1.50(2)
C(14)	C(15)	1.380(18)	C(14)	C(19)	1.459(14)
C(15)	C(20)	1.52(2)	C(26)	C(27)	1.411(18)
C(27)	C(28)	1.380(14)	C(28)	C(29)	1.372(16)
C(29)	C(30)	1.335(18)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(6)	H(1)	0.950	C(6)	H(2)	0.950
C(6)	H(3)	0.950	C(7)	H(4)	0.950
C(7)	H(5)	0.950	C(7)	H(6)	0.950
C(8)	H(7)	0.950	C(8)	H(8)	0.950
C(8)	H(9)	0.950	C(9)	H(10)	0.950
C(9)	H(11)	0.950	C(9)	H(12)	0.950
C(10)	H(13)	0.950	C(10)	H(14)	0.950
C(10)	H(15)	0.950	C(16)	H(16)	0.950
C(16)	H(17)	0.950	C(16)	H(18)	0.950
C(17)	H(19)	0.950	C(17)	H(20)	0.950
C(17)	H(21)	0.950	C(18)	H(22)	0.950
C(18)	H(23)	0.950	C(18)	H(24)	0.950
C(19)	H(25)	0.950	C(19)	H(26)	0.950
C(19)	H(27)	0.950	C(20)	H(28)	0.950
C(20)	H(29)	0.950	C(20)	H(30)	0.950
C(21)	H(31)	0.950	C(21)	H(32)	0.950
C(21)	H(33)	0.950	C(22)	H(34)	0.950
C(22)	H(35)	0.950	C(22)	H(36)	0.950
C(23)	H(37)	0.950	C(23)	H(38)	0.950
C(24)	H(39)	0.950	C(24)	H(40)	0.950
C(24)	H(41)	0.950	C(25)	H(42)	0.950
C(25)	H(43)	0.950	C(25)	H(44)	0.950
C(27)	H(45)	0.950	C(28)	H(46)	0.950
C(29)	H(47)	0.950	C(30)	H(48)	0.950

Table 6. Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Ir(1)	C(1)	144.5(3)	P(1)	Ir(1)	C(2)	109.4(3)
P(1)	Ir(1)	C(3)	98.3(3)	P(1)	Ir(1)	C(4)	119.4(3)
P(1)	Ir(1)	C(5)	155.6(3)	P(1)	Ir(1)	C(26)	84.1(2)
C(1)	Ir(1)	C(2)	36.2(4)	C(1)	Ir(1)	C(3)	59.3(4)
C(1)	Ir(1)	C(4)	59.8(5)	C(1)	Ir(1)	C(5)	36.5(5)
C(1)	Ir(1)	C(26)	131.3(4)	C(2)	Ir(1)	C(3)	35.7(4)
C(2)	Ir(1)	C(4)	60.4(5)	C(2)	Ir(1)	C(5)	61.4(4)
C(2)	Ir(1)	C(26)	164.2(4)	C(3)	Ir(1)	C(4)	36.1(4)
C(3)	Ir(1)	C(5)	60.5(4)	C(3)	Ir(1)	C(26)	136.9(4)
C(4)	Ir(1)	C(5)	36.3(4)	C(4)	Ir(1)	C(26)	106.3(4)
C(5)	Ir(1)	C(26)	103.0(4)	P(2)	Ir(2)	N(1)	94.23(19)
P(2)	Ir(2)	C(11)	166.7(3)	P(2)	Ir(2)	C(12)	133.4(3)
P(2)	Ir(2)	C(13)	103.4(3)	P(2)	Ir(2)	C(14)	107.4(2)
P(2)	Ir(2)	C(15)	136.9(2)	N(1)	Ir(2)	C(11)	98.5(4)
N(1)	Ir(2)	C(12)	130.1(4)	N(1)	Ir(2)	C(13)	157.8(4)
N(1)	Ir(2)	C(14)	123.2(3)	N(1)	Ir(2)	C(15)	96.0(4)
C(11)	Ir(2)	C(12)	36.1(5)	C(11)	Ir(2)	C(13)	63.3(4)
C(11)	Ir(2)	C(14)	62.0(3)	C(11)	Ir(2)	C(15)	37.7(3)
C(12)	Ir(2)	C(13)	39.5(4)	C(12)	Ir(2)	C(14)	63.4(3)
C(12)	Ir(2)	C(15)	61.5(3)	C(13)	Ir(2)	C(14)	38.3(4)
C(13)	Ir(2)	C(15)	61.8(4)	C(14)	Ir(2)	C(15)	35.2(4)
O(1)	S(1)	O(2)	114.1(8)	O(1)	S(1)	O(3)	112.9(8)
O(1)	S(1)	C(31)	99.2(8)	O(2)	S(1)	O(3)	120.3(7)
O(2)	S(1)	C(31)	102.7(7)	O(3)	S(1)	C(31)	103.9(8)
Ir(1)	P(1)	C(21)	115.9(5)	Ir(1)	P(1)	C(22)	116.7(4)
Ir(1)	P(1)	C(23)	117.8(2)	C(21)	P(1)	C(22)	100.9(6)
C(21)	P(1)	C(23)	100.5(5)	C(22)	P(1)	C(23)	102.3(5)
Ir(2)	P(2)	C(23)	112.9(3)	Ir(2)	P(2)	C(24)	120.7(4)
Ir(2)	P(2)	C(25)	113.4(3)	C(23)	P(2)	C(24)	106.6(4)
C(23)	P(2)	C(25)	101.4(5)	C(24)	P(2)	C(25)	99.5(6)

Ir(2)	N(1)	C(26)	130.5(6)	Ir(2)	N(1)	C(30)	109.9(6)
C(26)	N(1)	C(30)	119.4(9)	Ir(1)	C(1)	C(2)	71.6(6)
Ir(1)	C(1)	C(5)	72.8(7)	Ir(1)	C(1)	C(6)	129.1(9)
C(2)	C(1)	C(5)	110.1(11)	C(2)	C(1)	C(6)	123.1(15)
C(5)	C(1)	C(6)	126.2(13)	Ir(1)	C(2)	C(1)	72.2(5)
Ir(1)	C(2)	C(3)	73.4(6)	Ir(1)	C(2)	C(7)	129.2(10)
C(1)	C(2)	C(3)	107.2(12)	C(1)	C(2)	C(7)	125.1(13)
C(3)	C(2)	C(7)	126.6(10)	Ir(1)	C(3)	C(2)	70.9(5)
Ir(1)	C(3)	C(4)	71.9(6)	Ir(1)	C(3)	C(8)	128.0(9)
C(2)	C(3)	C(4)	108.9(10)	C(2)	C(3)	C(8)	127.5(12)
C(4)	C(3)	C(8)	123.4(13)	Ir(1)	C(4)	C(3)	72.0(8)
Ir(1)	C(4)	C(5)	72.0(8)	Ir(1)	C(4)	C(9)	132.0(9)
C(3)	C(4)	C(5)	108.4(12)	C(3)	C(4)	C(9)	123.1(11)
C(5)	C(4)	C(9)	127.2(13)	Ir(1)	C(5)	C(1)	70.7(7)
Ir(1)	C(5)	C(4)	71.7(8)	Ir(1)	C(5)	C(10)	128.8(8)
C(1)	C(5)	C(4)	105.3(10)	C(1)	C(5)	C(10)	128.3(12)
C(4)	C(5)	C(10)	125.7(14)	Ir(2)	C(11)	C(12)	70.3(5)
Ir(2)	C(11)	C(15)	71.9(5)	Ir(2)	C(11)	C(16)	126.2(9)
C(12)	C(11)	C(15)	107.3(10)	C(12)	C(11)	C(16)	128.5(10)
C(15)	C(11)	C(16)	124.1(12)	Ir(2)	C(12)	C(11)	73.6(5)
Ir(2)	C(12)	C(13)	69.5(5)	Ir(2)	C(12)	C(17)	129.3(8)
C(11)	C(12)	C(13)	108.6(9)	C(11)	C(12)	C(17)	125.4(11)
C(13)	C(12)	C(17)	125.5(13)	Ir(2)	C(13)	C(12)	71.0(6)
Ir(2)	C(13)	C(14)	75.3(6)	Ir(2)	C(13)	C(18)	127.6(8)
C(12)	C(13)	C(14)	106.4(11)	C(12)	C(13)	C(18)	125.8(10)
C(14)	C(13)	C(18)	126.8(10)	Ir(2)	C(14)	C(13)	66.4(5)
Ir(2)	C(14)	C(15)	70.9(5)	Ir(2)	C(14)	C(19)	127.2(6)
C(13)	C(14)	C(15)	106.3(8)	C(13)	C(14)	C(19)	123.6(12)
C(15)	C(14)	C(19)	130.1(11)	Ir(2)	C(15)	C(11)	70.4(5)
Ir(2)	C(15)	C(14)	73.9(5)	Ir(2)	C(15)	C(20)	126.1(7)
C(11)	C(15)	C(14)	111.3(10)	C(11)	C(15)	C(20)	123.4(11)
C(14)	C(15)	C(20)	125.2(9)	P(1)	C(23)	P(2)	116.9(4)
Ir(1)	C(26)	N(1)	127.3(8)	Ir(1)	C(26)	C(27)	116.2(6)

N(1)	C(26)	C(27)	116.4(7)	C(26)	C(27)	C(28)	123.5(10)
C(27)	C(28)	C(29)	117.2(12)	C(28)	C(29)	C(30)	120.0(9)
N(1)	C(30)	C(29)	123.2(9)	S(1)	C(31)	F(1)	113.9(11)
S(1)	C(31)	F(2)	110.8(11)	S(1)	C(31)	F(3)	112.0(11)
F(1)	C(31)	F(2)	106.9(14)	F(1)	C(31)	F(3)	108.7(14)
F(2)	C(31)	F(3)	103.9(13)				

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(6)	H(1)	110.1	C(1)	C(6)	H(2)	109.7
C(1)	C(6)	H(3)	108.5	H(1)	C(6)	H(2)	109.5
H(1)	C(6)	H(3)	109.5	H(2)	C(6)	H(3)	109.5
C(2)	C(7)	H(4)	108.0	C(2)	C(7)	H(5)	110.5
C(2)	C(7)	H(6)	109.9	H(4)	C(7)	H(5)	109.5
H(4)	C(7)	H(6)	109.5	H(5)	C(7)	H(6)	109.5
C(3)	C(8)	H(7)	111.5	C(3)	C(8)	H(8)	107.8
C(3)	C(8)	H(9)	109.1	H(7)	C(8)	H(8)	109.5
H(7)	C(8)	H(9)	109.5	H(8)	C(8)	H(9)	109.5
C(4)	C(9)	H(10)	107.6	C(4)	C(9)	H(11)	111.3
C(4)	C(9)	H(12)	109.5	H(10)	C(9)	H(11)	109.5
H(10)	C(9)	H(12)	109.5	H(11)	C(9)	H(12)	109.5
C(5)	C(10)	H(13)	108.4	C(5)	C(10)	H(14)	110.3
C(5)	C(10)	H(15)	109.7	H(13)	C(10)	H(14)	109.5
H(13)	C(10)	H(15)	109.5	H(14)	C(10)	H(15)	109.5
C(11)	C(16)	H(16)	108.2	C(11)	C(16)	H(17)	109.9
C(11)	C(16)	H(18)	110.3	H(16)	C(16)	H(17)	109.5
H(16)	C(16)	H(18)	109.5	H(17)	C(16)	H(18)	109.5
C(12)	C(17)	H(19)	109.7	C(12)	C(17)	H(20)	111.5
C(12)	C(17)	H(21)	107.2	H(19)	C(17)	H(20)	109.5
H(19)	C(17)	H(21)	109.5	H(20)	C(17)	H(21)	109.5
C(13)	C(18)	H(22)	108.8	C(13)	C(18)	H(23)	110.1
C(13)	C(18)	H(24)	109.5	H(22)	C(18)	H(23)	109.5
H(22)	C(18)	H(24)	109.5	H(23)	C(18)	H(24)	109.5
C(14)	C(19)	H(25)	108.2	C(14)	C(19)	H(26)	109.9
C(14)	C(19)	H(27)	110.3	H(25)	C(19)	H(26)	109.5
H(25)	C(19)	H(27)	109.5	H(26)	C(19)	H(27)	109.5
C(15)	C(20)	H(28)	111.1	C(15)	C(20)	H(29)	108.6
C(15)	C(20)	H(30)	108.6	H(28)	C(20)	H(29)	109.5
H(28)	C(20)	H(30)	109.5	H(29)	C(20)	H(30)	109.5

P(1)	C(21)	H(31)	110.1	P(1)	C(21)	H(32)	109.3
P(1)	C(21)	H(33)	109.0	H(31)	C(21)	H(32)	109.5
H(31)	C(21)	H(33)	109.5	H(32)	C(21)	H(33)	109.5
P(1)	C(22)	H(34)	108.8	P(1)	C(22)	H(35)	109.8
P(1)	C(22)	H(36)	109.8	H(34)	C(22)	H(35)	109.5
H(34)	C(22)	H(36)	109.5	H(35)	C(22)	H(36)	109.5
P(1)	C(23)	H(37)	107.6	P(1)	C(23)	H(38)	107.6
P(2)	C(23)	H(37)	107.6	P(2)	C(23)	H(38)	107.6
H(37)	C(23)	H(38)	109.5	P(2)	C(24)	H(39)	109.7
P(2)	C(24)	H(40)	110.2	P(2)	C(24)	H(41)	108.5
H(39)	C(24)	H(40)	109.5	H(39)	C(24)	H(41)	109.5
H(40)	C(24)	H(41)	109.5	P(2)	C(25)	H(42)	109.5
P(2)	C(25)	H(43)	109.2	P(2)	C(25)	H(44)	109.7
H(42)	C(25)	H(43)	109.5	H(42)	C(25)	H(44)	109.5
H(43)	C(25)	H(44)	109.5	C(26)	C(27)	H(45)	118.3
C(28)	C(27)	H(45)	118.2	C(27)	C(28)	H(46)	121.6
C(29)	C(28)	H(46)	121.2	C(28)	C(29)	H(47)	119.9
C(30)	C(29)	H(47)	120.0	N(1)	C(30)	H(48)	118.1
C(29)	C(30)	H(48)	118.7				