

Dinitrogen Complexes of Pincer-Ligated Iridium

Rajshekhar Ghosh, Mira Kanzelberger, Thomas J. Emge,
Gene S. Hall and Alan S. Goldman*

*Department of Chemistry and Chemical Biology,
Rutgers-The State University of New Jersey, Piscataway, New Jersey, 08854*

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I. Experimental Section

Raman Spectra of complexes 1 and 2: Room temperature (21 ± 1 °C) Raman spectra were obtained from a Renishaw (Renishaw Inc., Hoffman Estates, IL) System 1000 dispersive micro-Raman spectrometer. The system has a 785 nm diode laser for illuminating the sample and a holographic notch filter to minimize the Raleigh scattered laser line. The Raman photons were focused onto a 1200 l/mm holographic grating and sent to a Peltier CCD detector for analysis. The laser intensity at the sample was 25 mW and we used a 50x objective lens from a Leica microscope to project the laser (2 micron spot) onto the sample. The laser beam was focused onto the sample crystals thru a sealed-glass NMR tube. We used acetaminophen (ASTM Designation: E 1840 – 96) to calibrate the Raman spectrometer over the data collection range of 2150 to 1860 cm^{-1} at 2 cm^{-1} resolution. The micro-Raman spectrometer is equipped with a computer controlled x, y, z stage. Under the control of Renishaw Wire 2.0 data acquisition software, data collection consisted of 3, 20 second accumulations per spot that were co-added to form an averaged data point per sample. Three separate random locations in the NMR tube were sampled to determine sample homogeneity that was confirmed by analysis of the three Raman spectra.

Infrared Spectra for complex 1: Room temperature (21 ± 1 °C) attenuated total reflectance (ATR) FTIR spectra were recorded on a Bruker (Billerica, MA) Equinox55 spectrometer equipped with a DTGS detector and KBr beamsplitter. We used a Smiths Detection (Danbury, CT) single reflection DuraScope ATR attachment that had a diamond crystal and a KRS-5 focusing element. Spectra were collected by pressing the sample onto the 2-mm diameter diamond crystal with a pressure setting of 6 on the DuraScope. One-hundred co-added spectra were accumulated between 4,000 and 400 cm^{-1} at 4 cm^{-1} resolution using the Blackman-Harris 3-term apodization function. All spectra were normalized by subtracting out a background spectra collected before each sample analysis. Spectra were analyzed as is with no further spectral manipulations.

II. X-ray Structure Determinations. Data were collected on a Bruker Smart APEX CCD diffractometer with graphite monochromatized Mo K α radiation ($\lambda = 0.71073\text{\AA}$) at 100K. The data were corrected for Lorenz effects and polarization, and absorption, the latter by a multi-scan (SADABS)¹ method. The structures were solved by Patterson or direct methods (SHELXS86).² All non-hydrogen atoms were refined (SHELXL97)³ based upon F_{obs}^2 . All hydrogen atom coordinates were calculated with idealized geometries (SHELXL97). Scattering factors (f_0 , f' , f'') are as described in SHELXL97. Crystal data for the structures have been deposited in the Cambridge Crystallographic Data Center with numbers (compound numbers) CCDC- 616700 (complex **1**), CCDC- 616699 (complex **2**).

References

- (1) Bruker-AXS. SADABS, Bruker area detector scaling and absorption correction, v2.05, Bruker-AXS Inc., Madison, Wisconsin, 2003; SAINTplus, Bruker area detector data reduction program, v6.45, Bruker-AXS Inc., Madison, Wisconsin, 2003.
- (2) Sheldrick, G. M. SHELXS86, Program for the Solution of Crystal Structures, University of Göttingen, Germany, 1986.
- (3) Sheldrick, G. M. SHELXL97, Program for Crystal Structure Refinement, University of Göttingen, Germany, 1997.

III. Structural Data for 1

Figure S-1 : ORTEP Diagram of complex 1

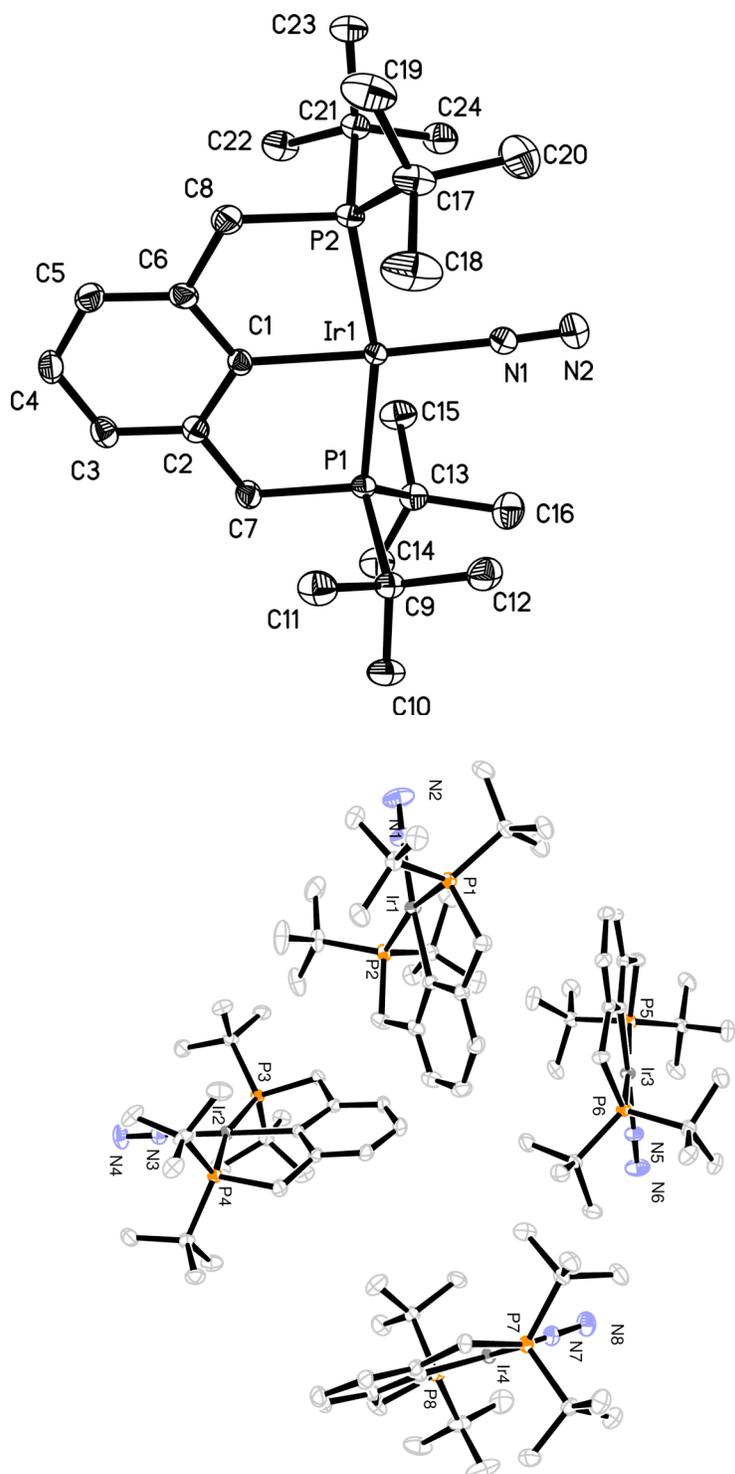


Table S-1. Crystal data and structure refinement for complex **1**.

Identification code	irn2zzz	
Empirical formula	C ₂₄ H ₄₃ Ir N ₂ P ₂	
Formula weight	613.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.2546(8) Å	α = 89.034(1)°.
	b = 15.8510(11) Å	β = 81.718(1)°.
	c = 29.533(2) Å	γ = 88.825(1)°.
Volume	5212.0(6) Å ³	
Z	8	
Density (calculated)	1.564 Mg/m ³	
Absorption coefficient	5.259 mm ⁻¹	
F(000)	2464	
Crystal size	0.30 x 0.11 x 0.10 mm ³	
Theta range for data collection	1.83 to 30.85°.	
Index ranges	-16 ≤ h ≤ 16, -22 ≤ k ≤ 22, -42 ≤ l ≤ 42	
Reflections collected	62903	
Independent reflections	31856 [R(int) = 0.0158]	
Completeness to theta = 30.85°	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9999 and 0.8068	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	31856 / 0 / 1093	
Goodness-of-fit on F ²	1.011	
Final R indices [I > 2σ(I)]	R1 = 0.0202, wR2 = 0.0421	
R indices (all data)	R1 = 0.0235, wR2 = 0.0431	
Largest diff. peak and hole	1.260 and -0.705 e.Å ⁻³	

Table S-2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for complex 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Ir(1)	5295(1)	1178(1)	6128(1)	14(1)
N(1)	4740(2)	367(1)	5719(1)	25(1)
N(2)	4396(2)	-118(2)	5509(1)	40(1)
P(1)	7161(1)	590(1)	6143(1)	15(1)
P(2)	3575(1)	1990(1)	6240(1)	15(1)
C(1)	5814(2)	1970(1)	6597(1)	15(1)
C(2)	6882(2)	1827(1)	6794(1)	17(1)
C(3)	7201(2)	2348(1)	7131(1)	21(1)
C(4)	6454(2)	3011(1)	7299(1)	23(1)
C(5)	5397(2)	3167(1)	7119(1)	22(1)
C(6)	5095(2)	2675(1)	6768(1)	18(1)
C(7)	7668(2)	1060(1)	6649(1)	19(1)
C(8)	3991(2)	2905(1)	6551(1)	22(1)
C(9)	8289(2)	911(1)	5642(1)	19(1)
C(10)	9538(2)	496(2)	5627(1)	27(1)
C(11)	8407(2)	1876(1)	5670(1)	28(1)
C(12)	7789(2)	727(2)	5196(1)	26(1)
C(13)	7272(2)	-577(1)	6267(1)	20(1)
C(14)	8425(2)	-860(1)	6452(1)	26(1)
C(15)	6198(2)	-766(1)	6636(1)	28(1)
C(16)	7152(2)	-1090(1)	5839(1)	29(1)
C(17)	3006(2)	2482(2)	5727(1)	25(1)
C(18)	4128(2)	2811(2)	5420(1)	43(1)
C(19)	2124(2)	3229(2)	5837(1)	35(1)
C(20)	2417(2)	1820(2)	5463(1)	38(1)
C(21)	2340(2)	1472(1)	6638(1)	17(1)
C(22)	2779(2)	1413(2)	7108(1)	26(1)
C(23)	1129(2)	1943(1)	6685(1)	24(1)
C(24)	2192(2)	570(1)	6477(1)	26(1)
Ir(2)	332(1)	6039(1)	6207(1)	13(1)
N(3)	-130(2)	6793(1)	5734(1)	21(1)
N(4)	-400(2)	7228(1)	5468(1)	31(1)
P(3)	-1379(1)	5255(1)	6316(1)	13(1)
P(4)	2128(1)	6644(1)	6268(1)	14(1)
C(25)	815(2)	5241(1)	6704(1)	14(1)
C(26)	110(2)	4537(1)	6872(1)	16(1)
C(27)	430(2)	4003(1)	7215(1)	19(1)
C(28)	1482(2)	4126(1)	7395(1)	22(1)
C(29)	2202(2)	4801(1)	7240(1)	20(1)
C(30)	1870(2)	5361(1)	6907(1)	16(1)
C(31)	-992(2)	4339(1)	6657(1)	18(1)
C(32)	2613(2)	6132(1)	6777(1)	19(1)
C(33)	-1906(2)	4754(1)	5810(1)	18(1)
C(34)	-2816(2)	4046(1)	5935(1)	23(1)
C(35)	-765(2)	4373(1)	5530(1)	25(1)
C(36)	-2440(2)	5417(1)	5510(1)	26(1)
C(37)	-2627(2)	5815(1)	6690(1)	17(1)
C(38)	-3839(2)	5373(1)	6748(1)	22(1)
C(39)	-2216(2)	5892(2)	7164(1)	26(1)
C(40)	-2768(2)	6713(1)	6498(1)	24(1)
C(41)	3356(2)	6393(1)	5789(1)	21(1)
C(42)	3526(2)	5426(2)	5799(1)	33(1)
C(43)	4555(2)	6810(2)	5823(1)	25(1)
C(44)	2947(2)	6636(2)	5330(1)	29(1)
C(45)	2100(2)	7799(1)	6410(1)	18(1)
C(46)	999(2)	7924(1)	6775(1)	26(1)
C(47)	3208(2)	8102(1)	6605(1)	24(1)
C(48)	1927(2)	8344(1)	5989(1)	27(1)
Ir(3)	1495(1)	1051(1)	8785(1)	13(1)

N(5)	604(2)	1782(1)	9243(1)	20(1)
N(6)	95(2)	2200(1)	9501(1)	30(1)
P(5)	-85(1)	248(1)	8647(1)	14(1)
P(6)	3341(1)	1639(1)	8783(1)	12(1)
C(49)	2432(2)	298(1)	8297(1)	13(1)
C(50)	1901(2)	-397(1)	8112(1)	14(1)
C(51)	2533(2)	-886(1)	7765(1)	16(1)
C(52)	3727(2)	-728(1)	7604(1)	18(1)
C(53)	4290(2)	-64(1)	7783(1)	17(1)
C(54)	3649(2)	449(1)	8116(1)	15(1)
C(55)	630(2)	-632(1)	8307(1)	17(1)
C(56)	4256(2)	1214(1)	8269(1)	16(1)
C(57)	-1064(2)	802(1)	8265(1)	18(1)
C(58)	-2180(2)	326(1)	8179(1)	25(1)
C(59)	-260(2)	950(2)	7806(1)	29(1)
C(60)	-1443(2)	1671(1)	8463(1)	24(1)
C(61)	-1008(2)	-295(1)	9145(1)	18(1)
C(62)	-1769(2)	-1022(1)	9011(1)	26(1)
C(63)	-101(2)	-657(2)	9444(1)	26(1)
C(64)	-1824(2)	348(1)	9429(1)	26(1)
C(65)	3479(2)	2811(1)	8696(1)	16(1)
C(66)	2715(2)	3034(1)	8317(1)	24(1)
C(67)	4764(2)	3113(1)	8534(1)	22(1)
C(68)	2954(2)	3284(1)	9129(1)	23(1)
C(69)	4121(2)	1260(1)	9271(1)	18(1)
C(70)	4267(2)	295(1)	9221(1)	28(1)
C(71)	5352(2)	1643(1)	9279(1)	23(1)
C(72)	3313(2)	1431(1)	9728(1)	23(1)
Ir(4)	6240(1)	6078(1)	8828(1)	13(1)
N(7)	5373(2)	5264(1)	9246(1)	19(1)
N(8)	4881(2)	4790(1)	9479(1)	29(1)
P(7)	8123(1)	5510(1)	8840(1)	14(1)
P(8)	4621(1)	6906(1)	8708(1)	15(1)
C(73)	7150(2)	6906(1)	8372(1)	15(1)
C(74)	8385(2)	6789(1)	8202(1)	16(1)
C(75)	8990(2)	7344(1)	7880(1)	20(1)
C(76)	8389(2)	8018(1)	7703(1)	24(1)
C(77)	7177(2)	8151(1)	7863(1)	23(1)
C(78)	6574(2)	7622(1)	8198(1)	18(1)
C(79)	9045(2)	6017(1)	8349(1)	17(1)
C(80)	5290(2)	7833(1)	8396(1)	24(1)
C(81)	8383(2)	4352(1)	8724(1)	18(1)
C(82)	9705(2)	4092(1)	8578(1)	23(1)
C(83)	7683(2)	4170(1)	8328(1)	25(1)
C(84)	7865(2)	3814(1)	9143(1)	26(1)
C(85)	8790(2)	5834(1)	9358(1)	18(1)
C(86)	10035(2)	5446(2)	9393(1)	25(1)
C(87)	8889(2)	6800(1)	9328(1)	27(1)
C(88)	7921(2)	5615(2)	9792(1)	24(1)
C(89)	3662(2)	6428(1)	8313(1)	18(1)
C(90)	4468(2)	6346(2)	7849(1)	30(1)
C(91)	2523(2)	6934(1)	8244(1)	27(1)
C(92)	3315(2)	5535(1)	8484(1)	24(1)
C(93)	3682(2)	7380(1)	9221(1)	26(1)
C(94)	2903(2)	8142(2)	9113(1)	37(1)
C(95)	2872(2)	6719(2)	9487(1)	38(1)
C(96)	4589(2)	7669(2)	9528(1)	47(1)

Table S-3. Bond lengths [Å] and angles [°] for complex 1.

Ir(1)-N(1)	1.9489(18)	Ir(3)-N(5)	1.9472(17)
Ir(1)-C(1)	2.0398(19)	Ir(3)-C(49)	2.0452(18)
Ir(1)-P(1)	2.2867(5)	Ir(3)-P(6)	2.2936(5)
Ir(1)-P(2)	2.2897(5)	Ir(3)-P(5)	2.2945(5)
N(1)-N(2)	1.107(3)	N(5)-N(6)	1.107(2)
P(1)-C(7)	1.846(2)	P(5)-C(55)	1.8367(19)
P(1)-C(9)	1.877(2)	P(5)-C(61)	1.8802(19)
P(1)-C(13)	1.883(2)	P(5)-C(57)	1.8825(19)
P(2)-C(8)	1.835(2)	P(6)-C(56)	1.8361(19)
P(2)-C(21)	1.8790(19)	P(6)-C(69)	1.877(2)
P(2)-C(17)	1.879(2)	P(6)-C(65)	1.8777(19)
C(1)-C(2)	1.421(3)	C(49)-C(50)	1.417(3)
C(1)-C(6)	1.422(3)	C(49)-C(54)	1.421(2)
C(2)-C(3)	1.396(3)	C(50)-C(51)	1.397(3)
C(2)-C(7)	1.518(3)	C(50)-C(55)	1.514(3)
C(3)-C(4)	1.386(3)	C(51)-C(52)	1.386(3)
C(4)-C(5)	1.388(3)	C(52)-C(53)	1.389(3)
C(5)-C(6)	1.391(3)	C(53)-C(54)	1.395(2)
C(6)-C(8)	1.514(3)	C(54)-C(56)	1.511(3)
C(9)-C(10)	1.535(3)	C(57)-C(58)	1.532(3)
C(9)-C(12)	1.540(3)	C(57)-C(59)	1.534(3)
C(9)-C(11)	1.542(3)	C(57)-C(60)	1.535(3)
C(13)-C(14)	1.536(3)	C(61)-C(64)	1.533(3)
C(13)-C(15)	1.537(3)	C(61)-C(63)	1.538(3)
C(13)-C(16)	1.538(3)	C(61)-C(62)	1.540(3)
C(17)-C(20)	1.534(4)	C(65)-C(68)	1.532(3)
C(17)-C(19)	1.538(3)	C(65)-C(66)	1.536(3)
C(17)-C(18)	1.541(3)	C(65)-C(67)	1.540(3)
C(21)-C(23)	1.530(3)	C(69)-C(71)	1.528(3)
C(21)-C(24)	1.535(3)	C(69)-C(72)	1.538(3)
C(21)-C(22)	1.538(3)	C(69)-C(70)	1.542(3)
Ir(2)-N(3)	1.9442(17)	Ir(4)-N(7)	1.9482(17)
Ir(2)-C(25)	2.0483(18)	Ir(4)-C(73)	2.0446(18)
Ir(2)-P(4)	2.2867(5)	Ir(4)-P(8)	2.2894(5)
Ir(2)-P(3)	2.2940(5)	Ir(4)-P(7)	2.2902(5)
N(3)-N(4)	1.107(2)	N(7)-N(8)	1.109(2)
P(3)-C(31)	1.8337(19)	P(7)-C(79)	1.8412(19)
P(3)-C(37)	1.8744(19)	P(7)-C(85)	1.880(2)
P(3)-C(33)	1.880(2)	P(7)-C(81)	1.883(2)
P(4)-C(32)	1.8411(19)	P(8)-C(80)	1.838(2)
P(4)-C(41)	1.872(2)	P(8)-C(93)	1.875(2)
P(4)-C(45)	1.883(2)	P(8)-C(89)	1.878(2)
C(25)-C(30)	1.421(3)	C(73)-C(74)	1.418(3)
C(25)-C(26)	1.422(3)	C(73)-C(78)	1.421(3)
C(26)-C(27)	1.392(3)	C(74)-C(75)	1.396(3)
C(26)-C(31)	1.511(3)	C(74)-C(79)	1.508(3)
C(27)-C(28)	1.385(3)	C(75)-C(76)	1.388(3)
C(28)-C(29)	1.386(3)	C(76)-C(77)	1.390(3)
C(29)-C(30)	1.399(3)	C(77)-C(78)	1.394(3)
C(30)-C(32)	1.509(3)	C(78)-C(80)	1.512(3)
C(33)-C(36)	1.531(3)	C(81)-C(83)	1.537(3)
C(33)-C(34)	1.540(3)	C(81)-C(82)	1.538(3)
C(33)-C(35)	1.541(3)	C(81)-C(84)	1.540(3)
C(37)-C(38)	1.533(3)	C(85)-C(86)	1.535(3)
C(37)-C(40)	1.536(3)	C(85)-C(88)	1.536(3)
C(37)-C(39)	1.545(3)	C(85)-C(87)	1.538(3)
C(41)-C(43)	1.532(3)	C(89)-C(92)	1.534(3)
C(41)-C(44)	1.534(3)	C(89)-C(91)	1.535(3)
C(41)-C(42)	1.542(3)	C(89)-C(90)	1.536(3)
C(45)-C(46)	1.532(3)	C(93)-C(95)	1.534(4)
C(45)-C(47)	1.535(3)	C(93)-C(94)	1.534(3)
C(45)-C(48)	1.537(3)	C(93)-C(96)	1.542(3)

N(1)-Ir(1)-C(1)	175.51(8)	N(4)-N(3)-Ir(2)	179.20(19)
N(1)-Ir(1)-P(1)	97.24(5)	C(31)-P(3)-C(37)	104.95(9)
C(1)-Ir(1)-P(1)	83.03(5)	C(31)-P(3)-C(33)	102.75(9)
N(1)-Ir(1)-P(2)	96.93(5)	C(37)-P(3)-C(33)	112.30(9)
C(1)-Ir(1)-P(2)	82.77(5)	C(31)-P(3)-Ir(2)	104.46(6)
P(1)-Ir(1)-P(2)	165.807(18)	C(37)-P(3)-Ir(2)	111.37(6)
N(2)-N(1)-Ir(1)	176.0(2)	C(33)-P(3)-Ir(2)	119.24(6)
C(7)-P(1)-C(9)	105.67(9)	C(32)-P(4)-C(41)	104.77(9)
C(7)-P(1)-C(13)	102.77(9)	C(32)-P(4)-C(45)	103.07(9)
C(9)-P(1)-C(13)	111.23(9)	C(41)-P(4)-C(45)	111.11(9)
C(7)-P(1)-Ir(1)	104.02(6)	C(32)-P(4)-Ir(2)	104.41(6)
C(9)-P(1)-Ir(1)	113.41(6)	C(41)-P(4)-Ir(2)	114.36(7)
C(13)-P(1)-Ir(1)	118.05(7)	C(45)-P(4)-Ir(2)	117.34(6)
C(8)-P(2)-C(21)	105.09(9)	C(30)-C(25)-C(26)	115.91(16)
C(8)-P(2)-C(17)	103.16(10)	C(30)-C(25)-Ir(2)	122.06(14)
C(21)-P(2)-C(17)	111.81(9)	C(26)-C(25)-Ir(2)	122.03(13)
C(8)-P(2)-Ir(1)	103.96(7)	C(27)-C(26)-C(25)	121.92(17)
C(21)-P(2)-Ir(1)	112.50(6)	C(27)-C(26)-C(31)	118.79(17)
C(17)-P(2)-Ir(1)	118.56(7)	C(25)-C(26)-C(31)	119.24(16)
C(2)-C(1)-C(6)	115.56(17)	C(28)-C(27)-C(26)	120.54(19)
C(2)-C(1)-Ir(1)	122.25(14)	C(27)-C(28)-C(29)	119.42(18)
C(6)-C(1)-Ir(1)	122.09(14)	C(28)-C(29)-C(30)	120.71(18)
C(3)-C(2)-C(1)	121.93(18)	C(29)-C(30)-C(25)	121.43(18)
C(3)-C(2)-C(7)	119.03(17)	C(29)-C(30)-C(32)	119.31(17)
C(1)-C(2)-C(7)	118.97(17)	C(25)-C(30)-C(32)	119.19(16)
C(4)-C(3)-C(2)	120.57(19)	C(26)-C(31)-P(3)	108.86(13)
C(3)-C(4)-C(5)	119.24(19)	C(30)-C(32)-P(4)	109.47(13)
C(4)-C(5)-C(6)	120.67(19)	C(36)-C(33)-C(34)	109.28(16)
C(5)-C(6)-C(1)	121.93(18)	C(36)-C(33)-C(35)	108.29(17)
C(5)-C(6)-C(8)	119.48(18)	C(34)-C(33)-C(35)	108.62(17)
C(1)-C(6)-C(8)	118.56(17)	C(36)-C(33)-P(3)	111.05(14)
C(2)-C(7)-P(1)	109.23(13)	C(34)-C(33)-P(3)	114.17(14)
C(6)-C(8)-P(2)	108.77(13)	C(35)-C(33)-P(3)	105.18(13)
C(10)-C(9)-C(12)	109.54(17)	C(38)-C(37)-C(40)	109.81(16)
C(10)-C(9)-C(11)	108.93(17)	C(38)-C(37)-C(39)	108.77(17)
C(12)-C(9)-C(11)	107.51(17)	C(40)-C(37)-C(39)	107.59(17)
C(10)-C(9)-P(1)	115.06(14)	C(38)-C(37)-P(3)	115.09(14)
C(12)-C(9)-P(1)	109.17(14)	C(40)-C(37)-P(3)	108.77(13)
C(11)-C(9)-P(1)	106.34(14)	C(39)-C(37)-P(3)	106.52(13)
C(14)-C(13)-C(15)	108.16(17)	C(43)-C(41)-C(44)	109.49(18)
C(14)-C(13)-C(16)	108.98(17)	C(43)-C(41)-C(42)	109.43(18)
C(15)-C(13)-C(16)	108.70(18)	C(44)-C(41)-C(42)	107.32(18)
C(14)-C(13)-P(1)	114.53(14)	C(43)-C(41)-P(4)	114.65(14)
C(15)-C(13)-P(1)	105.35(14)	C(44)-C(41)-P(4)	109.71(14)
C(16)-C(13)-P(1)	110.89(14)	C(42)-C(41)-P(4)	105.96(15)
C(20)-C(17)-C(19)	109.16(19)	C(46)-C(45)-C(47)	108.26(17)
C(20)-C(17)-C(18)	108.7(2)	C(46)-C(45)-C(48)	108.46(17)
C(19)-C(17)-C(18)	108.1(2)	C(47)-C(45)-C(48)	108.95(17)
C(20)-C(17)-P(2)	110.82(15)	C(46)-C(45)-P(4)	105.30(14)
C(19)-C(17)-P(2)	114.48(16)	C(47)-C(45)-P(4)	115.04(14)
C(18)-C(17)-P(2)	105.39(15)	C(48)-C(45)-P(4)	110.58(14)
C(23)-C(21)-C(24)	109.59(17)	N(5)-Ir(3)-C(49)	179.14(7)
C(23)-C(21)-C(22)	109.51(17)	N(5)-Ir(3)-P(6)	97.16(5)
C(24)-C(21)-C(22)	107.78(17)	C(49)-Ir(3)-P(6)	82.63(5)
C(23)-C(21)-P(2)	114.69(14)	N(5)-Ir(3)-P(5)	97.47(5)
C(24)-C(21)-P(2)	108.92(14)	C(49)-Ir(3)-P(5)	82.74(5)
C(22)-C(21)-P(2)	106.09(13)	P(6)-Ir(3)-P(5)	165.370(17)
N(3)-Ir(2)-C(25)	179.79(6)	N(6)-N(5)-Ir(3)	179.63(18)
N(3)-Ir(2)-P(4)	97.20(5)	C(55)-P(5)-C(61)	103.36(9)
C(25)-Ir(2)-P(4)	82.98(5)	C(55)-P(5)-C(57)	104.87(9)
N(3)-Ir(2)-P(3)	97.38(5)	C(61)-P(5)-C(57)	111.46(9)
C(25)-Ir(2)-P(3)	82.45(5)	C(55)-P(5)-Ir(3)	104.07(6)
P(4)-Ir(2)-P(3)	165.110(17)	C(61)-P(5)-Ir(3)	118.57(7)

C(57)-P(5)-Ir(3)	112.75(6)	N(8)-N(7)-Ir(4)	178.84(19)
C(56)-P(6)-C(69)	104.82(9)	C(79)-P(7)-C(85)	105.50(9)
C(56)-P(6)-C(65)	103.10(9)	C(79)-P(7)-C(81)	103.04(9)
C(69)-P(6)-C(65)	111.18(9)	C(85)-P(7)-C(81)	111.43(9)
C(56)-P(6)-Ir(3)	104.20(6)	C(79)-P(7)-Ir(4)	104.05(6)
C(69)-P(6)-Ir(3)	113.23(6)	C(85)-P(7)-Ir(4)	112.38(6)
C(65)-P(6)-Ir(3)	118.51(6)	C(81)-P(7)-Ir(4)	118.78(6)
C(50)-C(49)-C(54)	115.84(16)	C(80)-P(8)-C(93)	102.99(11)
C(50)-C(49)-Ir(3)	122.13(13)	C(80)-P(8)-C(89)	105.01(10)
C(54)-C(49)-Ir(3)	122.02(13)	C(93)-P(8)-C(89)	111.46(9)
C(51)-C(50)-C(49)	121.71(17)	C(80)-P(8)-Ir(4)	104.06(7)
C(51)-C(50)-C(55)	119.18(17)	C(93)-P(8)-Ir(4)	117.83(7)
C(49)-C(50)-C(55)	119.08(16)	C(89)-P(8)-Ir(4)	113.68(6)
C(52)-C(51)-C(50)	120.59(18)	C(74)-C(73)-C(78)	115.94(17)
C(51)-C(52)-C(53)	119.54(17)	C(74)-C(73)-Ir(4)	122.07(13)
C(52)-C(53)-C(54)	120.11(18)	C(78)-C(73)-Ir(4)	121.96(14)
C(53)-C(54)-C(49)	122.14(17)	C(75)-C(74)-C(73)	121.69(18)
C(53)-C(54)-C(56)	118.55(16)	C(75)-C(74)-C(79)	118.93(17)
C(49)-C(54)-C(56)	119.23(16)	C(73)-C(74)-C(79)	119.28(16)
C(50)-C(55)-P(5)	109.06(13)	C(76)-C(75)-C(74)	120.85(19)
C(54)-C(56)-P(6)	109.00(12)	C(75)-C(76)-C(77)	118.90(19)
C(58)-C(57)-C(59)	108.87(18)	C(76)-C(77)-C(78)	120.79(19)
C(58)-C(57)-C(60)	109.51(17)	C(77)-C(78)-C(73)	121.71(19)
C(59)-C(57)-C(60)	107.27(17)	C(77)-C(78)-C(80)	119.34(18)
C(58)-C(57)-P(5)	115.89(14)	C(73)-C(78)-C(80)	118.91(17)
C(59)-C(57)-P(5)	105.94(13)	C(74)-C(79)-P(7)	109.15(13)
C(60)-C(57)-P(5)	109.00(14)	C(78)-C(80)-P(8)	109.07(13)
C(64)-C(61)-C(63)	108.24(18)	C(83)-C(81)-C(82)	108.27(17)
C(64)-C(61)-C(62)	109.50(17)	C(83)-C(81)-C(84)	108.59(17)
C(63)-C(61)-C(62)	108.58(17)	C(82)-C(81)-C(84)	109.04(16)
C(64)-C(61)-P(5)	110.21(13)	C(83)-C(81)-P(7)	105.14(13)
C(63)-C(61)-P(5)	105.67(13)	C(82)-C(81)-P(7)	114.62(14)
C(62)-C(61)-P(5)	114.40(14)	C(84)-C(81)-P(7)	110.96(14)
C(68)-C(65)-C(66)	108.47(16)	C(86)-C(85)-C(88)	109.64(16)
C(68)-C(65)-C(67)	109.24(16)	C(86)-C(85)-C(87)	108.93(17)
C(66)-C(65)-C(67)	107.89(16)	C(88)-C(85)-C(87)	107.64(17)
C(68)-C(65)-P(6)	111.13(13)	C(86)-C(85)-P(7)	114.62(14)
C(66)-C(65)-P(6)	105.06(13)	C(88)-C(85)-P(7)	109.39(14)
C(67)-C(65)-P(6)	114.75(13)	C(87)-C(85)-P(7)	106.36(14)
C(71)-C(69)-C(72)	109.53(17)	C(92)-C(89)-C(91)	109.31(17)
C(71)-C(69)-C(70)	109.25(17)	C(92)-C(89)-C(90)	107.66(18)
C(72)-C(69)-C(70)	107.56(17)	C(91)-C(89)-C(90)	108.84(17)
C(71)-C(69)-P(6)	114.43(14)	C(92)-C(89)-P(8)	109.20(13)
C(72)-C(69)-P(6)	109.72(13)	C(91)-C(89)-P(8)	115.68(14)
C(70)-C(69)-P(6)	106.08(14)	C(90)-C(89)-P(8)	105.84(14)
N(7)-Ir(4)-C(73)	178.16(7)	C(95)-C(93)-C(94)	108.72(19)
N(7)-Ir(4)-P(8)	97.32(5)	C(95)-C(93)-C(96)	108.3(2)
C(73)-Ir(4)-P(8)	82.95(5)	C(94)-C(93)-C(96)	108.7(2)
N(7)-Ir(4)-P(7)	97.07(5)	C(95)-C(93)-P(8)	111.23(15)
C(73)-Ir(4)-P(7)	82.71(5)	C(94)-C(93)-P(8)	114.61(17)
P(8)-Ir(4)-P(7)	165.541(17)	C(96)-C(93)-P(8)	105.11(15)

Table S-4. Torsion angles [°] for complex 1.

C(1)-Ir(1)-N(1)-N(2)	2(3)	Ir(1)-P(1)-C(13)-C(14)	-157.50(13)
P(1)-Ir(1)-N(1)-N(2)	95(3)	C(7)-P(1)-C(13)-C(15)	74.94(16)
P(2)-Ir(1)-N(1)-N(2)	-84(3)	C(9)-P(1)-C(13)-C(15)	-172.41(14)
N(1)-Ir(1)-P(1)-C(7)	-162.88(9)	Ir(1)-P(1)-C(13)-C(15)	-38.78(16)
C(1)-Ir(1)-P(1)-C(7)	12.61(9)	C(7)-P(1)-C(13)-C(16)	-167.62(15)
P(2)-Ir(1)-P(1)-C(7)	13.57(11)	C(9)-P(1)-C(13)-C(16)	-54.97(17)
N(1)-Ir(1)-P(1)-C(9)	82.83(9)	Ir(1)-P(1)-C(13)-C(16)	78.66(15)
C(1)-Ir(1)-P(1)-C(9)	-101.69(9)	C(8)-P(2)-C(17)-C(20)	-170.61(16)
P(2)-Ir(1)-P(1)-C(9)	-100.73(10)	C(21)-P(2)-C(17)-C(20)	-58.19(18)
N(1)-Ir(1)-P(1)-C(13)	-49.85(10)	Ir(1)-P(2)-C(17)-C(20)	75.22(17)
C(1)-Ir(1)-P(1)-C(13)	125.64(9)	C(8)-P(2)-C(17)-C(19)	-46.64(18)
P(2)-Ir(1)-P(1)-C(13)	126.60(10)	C(21)-P(2)-C(17)-C(19)	65.78(19)
N(1)-Ir(1)-P(2)-C(8)	-171.44(9)	Ir(1)-P(2)-C(17)-C(19)	-160.81(14)
C(1)-Ir(1)-P(2)-C(8)	13.07(9)	C(8)-P(2)-C(17)-C(18)	72.02(19)
P(1)-Ir(1)-P(2)-C(8)	12.11(11)	C(21)-P(2)-C(17)-C(18)	-175.55(17)
N(1)-Ir(1)-P(2)-C(21)	75.41(9)	Ir(1)-P(2)-C(17)-C(18)	-42.1(2)
C(1)-Ir(1)-P(2)-C(21)	-100.08(9)	C(8)-P(2)-C(21)-C(23)	73.81(17)
P(1)-Ir(1)-P(2)-C(21)	-101.04(10)	C(17)-P(2)-C(21)-C(23)	-37.41(18)
N(1)-Ir(1)-P(2)-C(17)	-57.71(10)	Ir(1)-P(2)-C(21)-C(23)	-173.73(13)
C(1)-Ir(1)-P(2)-C(17)	126.80(10)	C(8)-P(2)-C(21)-C(24)	-162.99(14)
P(1)-Ir(1)-P(2)-C(17)	125.85(10)	C(17)-P(2)-C(21)-C(24)	85.80(16)
N(1)-Ir(1)-C(1)-C(2)	84.8(10)	Ir(1)-P(2)-C(21)-C(24)	-50.52(15)
P(1)-Ir(1)-C(1)-C(2)	-9.02(14)	C(8)-P(2)-C(21)-C(22)	-47.21(16)
P(2)-Ir(1)-C(1)-C(2)	171.22(15)	C(17)-P(2)-C(21)-C(22)	-158.42(14)
N(1)-Ir(1)-C(1)-C(6)	-91.5(10)	Ir(1)-P(2)-C(21)-C(22)	65.26(14)
P(1)-Ir(1)-C(1)-C(6)	174.74(15)	C(25)-Ir(2)-N(3)-N(4)	114(29)
P(2)-Ir(1)-C(1)-C(6)	-5.02(14)	P(4)-Ir(2)-N(3)-N(4)	-98(13)
C(6)-C(1)-C(2)-C(3)	-0.3(3)	P(3)-Ir(2)-N(3)-N(4)	78(13)
Ir(1)-C(1)-C(2)-C(3)	-176.74(15)	N(3)-Ir(2)-P(3)-C(31)	167.14(9)
C(6)-C(1)-C(2)-C(7)	176.73(17)	C(25)-Ir(2)-P(3)-C(31)	-12.74(8)
Ir(1)-C(1)-C(2)-C(7)	0.3(2)	P(4)-Ir(2)-P(3)-C(31)	-24.79(10)
C(1)-C(2)-C(3)-C(4)	2.5(3)	N(3)-Ir(2)-P(3)-C(37)	-80.09(9)
C(7)-C(2)-C(3)-C(4)	-174.54(19)	C(25)-Ir(2)-P(3)-C(37)	100.03(8)
C(2)-C(3)-C(4)-C(5)	-1.8(3)	P(4)-Ir(2)-P(3)-C(37)	87.98(9)
C(3)-C(4)-C(5)-C(6)	-1.0(3)	N(3)-Ir(2)-P(3)-C(33)	53.22(9)
C(4)-C(5)-C(6)-C(1)	3.3(3)	C(25)-Ir(2)-P(3)-C(33)	-126.66(9)
C(4)-C(5)-C(6)-C(8)	-174.87(19)	P(4)-Ir(2)-P(3)-C(33)	-138.71(9)
C(2)-C(1)-C(6)-C(5)	-2.6(3)	N(3)-Ir(2)-P(4)-C(32)	170.50(9)
Ir(1)-C(1)-C(6)-C(5)	173.90(15)	C(25)-Ir(2)-P(4)-C(32)	-9.61(9)
C(2)-C(1)-C(6)-C(8)	175.62(17)	P(3)-Ir(2)-P(4)-C(32)	2.43(11)
Ir(1)-C(1)-C(6)-C(8)	-7.9(2)	N(3)-Ir(2)-P(4)-C(41)	-75.59(9)
C(3)-C(2)-C(7)-P(1)	-171.54(15)	C(25)-Ir(2)-P(4)-C(41)	104.30(9)
C(1)-C(2)-C(7)-P(1)	11.4(2)	P(3)-Ir(2)-P(4)-C(41)	116.34(10)
C(9)-P(1)-C(7)-C(2)	103.87(14)	N(3)-Ir(2)-P(4)-C(45)	57.19(9)
C(13)-P(1)-C(7)-C(2)	-139.44(14)	C(25)-Ir(2)-P(4)-C(45)	-122.92(9)
Ir(1)-P(1)-C(7)-C(2)	-15.83(15)	P(3)-Ir(2)-P(4)-C(45)	-110.88(9)
C(5)-C(6)-C(8)-P(2)	-162.72(16)	N(3)-Ir(2)-C(25)-C(30)	152(100)
C(1)-C(6)-C(8)-P(2)	19.0(2)	P(4)-Ir(2)-C(25)-C(30)	4.45(14)
C(21)-P(2)-C(8)-C(6)	98.38(15)	P(3)-Ir(2)-C(25)-C(30)	-172.46(15)
C(17)-P(2)-C(8)-C(6)	-144.34(14)	N(3)-Ir(2)-C(25)-C(26)	-28(26)
Ir(1)-P(2)-C(8)-C(6)	-20.00(15)	P(4)-Ir(2)-C(25)-C(26)	-176.13(15)
C(7)-P(1)-C(9)-C(10)	69.55(17)	P(3)-Ir(2)-C(25)-C(26)	6.97(14)
C(13)-P(1)-C(9)-C(10)	-41.25(18)	C(30)-C(25)-C(26)-C(27)	0.5(3)
Ir(1)-P(1)-C(9)-C(10)	-177.14(13)	Ir(2)-C(25)-C(26)-C(27)	-178.95(14)
C(7)-P(1)-C(9)-C(12)	-166.84(14)	C(30)-C(25)-C(26)-C(31)	-176.84(17)
C(13)-P(1)-C(9)-C(12)	82.36(16)	Ir(2)-C(25)-C(26)-C(31)	3.7(2)
Ir(1)-P(1)-C(9)-C(12)	-53.53(15)	C(25)-C(26)-C(27)-C(28)	-2.4(3)
C(7)-P(1)-C(9)-C(11)	-51.12(16)	C(31)-C(26)-C(27)-C(28)	174.99(18)
C(13)-P(1)-C(9)-C(11)	-161.93(14)	C(26)-C(27)-C(28)-C(29)	1.8(3)
Ir(1)-P(1)-C(9)-C(11)	62.19(15)	C(27)-C(28)-C(29)-C(30)	0.5(3)
C(7)-P(1)-C(13)-C(14)	-43.78(17)	C(28)-C(29)-C(30)-C(25)	-2.4(3)
C(9)-P(1)-C(13)-C(14)	68.87(17)	C(28)-C(29)-C(30)-C(32)	174.44(19)

C(26)-C(25)-C(30)-C(29)	1.9(3)	P(5)-Ir(3)-P(6)-C(56)	12.62(10)
Ir(2)-C(25)-C(30)-C(29)	-178.68(14)	N(5)-Ir(3)-P(6)-C(69)	80.28(9)
C(26)-C(25)-C(30)-C(32)	-175.00(17)	C(49)-Ir(3)-P(6)-C(69)	-100.55(8)
Ir(2)-C(25)-C(30)-C(32)	4.5(2)	P(5)-Ir(3)-P(6)-C(69)	-100.70(9)
C(27)-C(26)-C(31)-P(3)	167.60(15)	N(5)-Ir(3)-P(6)-C(65)	-52.60(9)
C(25)-C(26)-C(31)-P(3)	-15.0(2)	C(49)-Ir(3)-P(6)-C(65)	126.56(9)
C(37)-P(3)-C(31)-C(26)	-99.57(14)	P(5)-Ir(3)-P(6)-C(65)	126.42(9)
C(33)-P(3)-C(31)-C(26)	142.85(13)	N(5)-Ir(3)-C(49)-C(50)	-110(5)
Ir(2)-P(3)-C(31)-C(26)	17.71(14)	P(6)-Ir(3)-C(49)-C(50)	174.02(15)
C(29)-C(30)-C(32)-P(4)	170.25(15)	P(5)-Ir(3)-C(49)-C(50)	-6.01(14)
C(25)-C(30)-C(32)-P(4)	-12.8(2)	N(5)-Ir(3)-C(49)-C(54)	68(5)
C(41)-P(4)-C(32)-C(30)	-106.39(15)	P(6)-Ir(3)-C(49)-C(54)	-7.25(14)
C(45)-P(4)-C(32)-C(30)	137.28(14)	P(5)-Ir(3)-C(49)-C(54)	172.72(15)
Ir(2)-P(4)-C(32)-C(30)	14.16(15)	C(54)-C(49)-C(50)-C(51)	-1.5(3)
C(31)-P(3)-C(33)-C(36)	172.15(15)	Ir(3)-C(49)-C(50)-C(51)	177.27(14)
C(37)-P(3)-C(33)-C(36)	59.90(17)	C(54)-C(49)-C(50)-C(55)	176.33(16)
Ir(2)-P(3)-C(33)-C(36)	-73.01(15)	Ir(3)-C(49)-C(50)-C(55)	-4.9(2)
C(31)-P(3)-C(33)-C(34)	48.06(16)	C(49)-C(50)-C(51)-C(52)	2.9(3)
C(37)-P(3)-C(33)-C(34)	-64.19(16)	C(55)-C(50)-C(51)-C(52)	-175.00(17)
Ir(2)-P(3)-C(33)-C(34)	162.90(12)	C(50)-C(51)-C(52)-C(53)	-1.4(3)
C(31)-P(3)-C(33)-C(35)	-70.92(15)	C(51)-C(52)-C(53)-C(54)	-1.2(3)
C(37)-P(3)-C(33)-C(35)	176.83(13)	C(52)-C(53)-C(54)-C(49)	2.5(3)
Ir(2)-P(3)-C(33)-C(35)	43.92(15)	C(52)-C(53)-C(54)-C(56)	-174.19(17)
C(31)-P(3)-C(37)-C(38)	-72.56(16)	C(50)-C(49)-C(54)-C(53)	-1.1(3)
C(33)-P(3)-C(37)-C(38)	38.31(17)	Ir(3)-C(49)-C(54)-C(53)	-179.94(14)
Ir(2)-P(3)-C(37)-C(38)	174.98(13)	C(50)-C(49)-C(54)-C(56)	175.55(16)
C(31)-P(3)-C(37)-C(40)	163.77(14)	Ir(3)-C(49)-C(54)-C(56)	-3.2(2)
C(33)-P(3)-C(37)-C(40)	-85.35(15)	C(51)-C(50)-C(55)-P(5)	-166.52(14)
Ir(2)-P(3)-C(37)-C(40)	51.32(14)	C(49)-C(50)-C(55)-P(5)	15.6(2)
C(31)-P(3)-C(37)-C(39)	48.06(15)	C(61)-P(5)-C(55)-C(50)	-142.04(13)
C(33)-P(3)-C(37)-C(39)	158.94(13)	C(57)-P(5)-C(55)-C(50)	101.08(14)
Ir(2)-P(3)-C(37)-C(39)	-64.40(14)	Ir(3)-P(5)-C(55)-C(50)	-17.54(14)
C(32)-P(4)-C(41)-C(43)	-67.40(17)	C(53)-C(54)-C(56)-P(6)	-168.56(14)
C(45)-P(4)-C(41)-C(43)	43.23(18)	C(49)-C(54)-C(56)-P(6)	14.6(2)
Ir(2)-P(4)-C(41)-C(43)	178.90(13)	C(69)-P(6)-C(56)-C(54)	101.64(14)
C(32)-P(4)-C(41)-C(44)	168.94(15)	C(65)-P(6)-C(56)-C(54)	-141.91(13)
C(45)-P(4)-C(41)-C(44)	-80.43(17)	Ir(3)-P(6)-C(56)-C(54)	-17.55(14)
Ir(2)-P(4)-C(41)-C(44)	55.24(17)	C(55)-P(5)-C(57)-C(58)	70.73(17)
C(32)-P(4)-C(41)-C(42)	53.39(16)	C(61)-P(5)-C(57)-C(58)	-40.45(18)
C(45)-P(4)-C(41)-C(42)	164.03(14)	Ir(3)-P(5)-C(57)-C(58)	-176.68(13)
Ir(2)-P(4)-C(41)-C(42)	-60.31(15)	C(55)-P(5)-C(57)-C(59)	-50.10(16)
C(32)-P(4)-C(45)-C(46)	-72.98(15)	C(61)-P(5)-C(57)-C(59)	-161.27(14)
C(41)-P(4)-C(45)-C(46)	175.29(13)	Ir(3)-P(5)-C(57)-C(59)	62.50(15)
Ir(2)-P(4)-C(45)-C(46)	41.08(15)	C(55)-P(5)-C(57)-C(60)	-165.24(13)
C(32)-P(4)-C(45)-C(47)	46.12(16)	C(61)-P(5)-C(57)-C(60)	83.58(15)
C(41)-P(4)-C(45)-C(47)	-65.60(17)	Ir(3)-P(5)-C(57)-C(60)	-52.65(14)
Ir(2)-P(4)-C(45)-C(47)	160.18(12)	C(55)-P(5)-C(61)-C(64)	-171.23(15)
C(32)-P(4)-C(45)-C(48)	170.06(15)	C(57)-P(5)-C(61)-C(64)	-59.09(17)
C(41)-P(4)-C(45)-C(48)	58.34(16)	Ir(3)-P(5)-C(61)-C(64)	74.32(15)
Ir(2)-P(4)-C(45)-C(48)	-75.88(15)	C(55)-P(5)-C(61)-C(63)	72.05(15)
C(49)-Ir(3)-N(5)-N(6)	22(31)	C(57)-P(5)-C(61)-C(63)	-175.82(14)
P(6)-Ir(3)-N(5)-N(6)	98(29)	Ir(3)-P(5)-C(61)-C(63)	-42.40(15)
P(5)-Ir(3)-N(5)-N(6)	-82(29)	C(55)-P(5)-C(61)-C(62)	-47.34(16)
N(5)-Ir(3)-P(5)-C(55)	-168.65(8)	C(57)-P(5)-C(61)-C(62)	64.80(16)
C(49)-Ir(3)-P(5)-C(55)	12.19(8)	Ir(3)-P(5)-C(61)-C(62)	-161.79(12)
P(6)-Ir(3)-P(5)-C(55)	12.33(10)	C(56)-P(6)-C(65)-C(68)	-170.03(14)
N(5)-Ir(3)-P(5)-C(61)	-54.59(9)	C(69)-P(6)-C(65)-C(68)	-58.20(16)
C(49)-Ir(3)-P(5)-C(61)	126.25(9)	Ir(3)-P(6)-C(65)-C(68)	75.57(15)
P(6)-Ir(3)-P(5)-C(61)	126.39(9)	C(56)-P(6)-C(65)-C(66)	72.85(14)
N(5)-Ir(3)-P(5)-C(57)	78.26(9)	C(69)-P(6)-C(65)-C(66)	-175.31(13)
C(49)-Ir(3)-P(5)-C(57)	-100.90(9)	Ir(3)-P(6)-C(65)-C(66)	-41.54(15)
P(6)-Ir(3)-P(5)-C(57)	-100.76(9)	C(56)-P(6)-C(65)-C(67)	-45.47(16)
N(5)-Ir(3)-P(6)-C(56)	-166.41(8)	C(69)-P(6)-C(65)-C(67)	66.36(16)
C(49)-Ir(3)-P(6)-C(56)	12.76(8)	Ir(3)-P(6)-C(65)-C(67)	-159.87(12)

C(56)-P(6)-C(69)-C(71)	67.24(16)	C(74)-C(73)-C(78)-C(80)	-174.42(17)
C(65)-P(6)-C(69)-C(71)	-43.49(17)	Ir(4)-C(73)-C(78)-C(80)	7.2(3)
Ir(3)-P(6)-C(69)-C(71)	-179.82(12)	C(75)-C(74)-C(79)-P(7)	170.31(15)
C(56)-P(6)-C(69)-C(72)	-169.19(14)	C(73)-C(74)-C(79)-P(7)	-13.3(2)
C(65)-P(6)-C(69)-C(72)	80.07(16)	C(85)-P(7)-C(79)-C(74)	-101.56(14)
Ir(3)-P(6)-C(69)-C(72)	-56.26(15)	C(81)-P(7)-C(79)-C(74)	141.48(14)
C(56)-P(6)-C(69)-C(70)	-53.28(16)	Ir(4)-P(7)-C(79)-C(74)	16.91(14)
C(65)-P(6)-C(69)-C(70)	-164.01(14)	C(77)-C(78)-C(80)-P(8)	165.47(16)
Ir(3)-P(6)-C(69)-C(70)	59.66(15)	C(73)-C(78)-C(80)-P(8)	-17.1(2)
C(73)-Ir(4)-N(7)-N(8)	8(10)	C(93)-P(8)-C(80)-C(78)	141.29(15)
P(8)-Ir(4)-N(7)-N(8)	107(8)	C(89)-P(8)-C(80)-C(78)	-101.93(15)
P(7)-Ir(4)-N(7)-N(8)	-75(8)	Ir(4)-P(8)-C(80)-C(78)	17.80(16)
N(7)-Ir(4)-P(7)-C(79)	165.44(9)	C(79)-P(7)-C(81)-C(83)	-73.00(14)
C(73)-Ir(4)-P(7)-C(79)	-12.72(9)	C(85)-P(7)-C(81)-C(83)	174.33(13)
P(8)-Ir(4)-P(7)-C(79)	-20.33(11)	Ir(4)-P(7)-C(81)-C(83)	41.31(15)
N(7)-Ir(4)-P(7)-C(85)	-80.92(9)	C(79)-P(7)-C(81)-C(82)	45.77(16)
C(73)-Ir(4)-P(7)-C(85)	100.92(9)	C(85)-P(7)-C(81)-C(82)	-66.91(16)
P(8)-Ir(4)-P(7)-C(85)	93.31(10)	Ir(4)-P(7)-C(81)-C(82)	160.07(12)
N(7)-Ir(4)-P(7)-C(81)	51.68(9)	C(79)-P(7)-C(81)-C(84)	169.80(15)
C(73)-Ir(4)-P(7)-C(81)	-126.48(9)	C(85)-P(7)-C(81)-C(84)	57.12(17)
P(8)-Ir(4)-P(7)-C(81)	-134.09(9)	Ir(4)-P(7)-C(81)-C(84)	-75.90(15)
N(7)-Ir(4)-P(8)-C(80)	170.29(9)	C(79)-P(7)-C(85)-C(86)	-69.34(16)
C(73)-Ir(4)-P(8)-C(80)	-11.55(9)	C(81)-P(7)-C(85)-C(86)	41.78(17)
P(7)-Ir(4)-P(8)-C(80)	-3.94(11)	Ir(4)-P(7)-C(85)-C(86)	177.91(13)
N(7)-Ir(4)-P(8)-C(93)	57.06(10)	C(79)-P(7)-C(85)-C(88)	167.07(14)
C(73)-Ir(4)-P(8)-C(93)	-124.77(10)	C(81)-P(7)-C(85)-C(88)	-81.81(15)
P(7)-Ir(4)-P(8)-C(93)	-117.16(11)	Ir(4)-P(7)-C(85)-C(88)	54.32(15)
N(7)-Ir(4)-P(8)-C(89)	-76.04(9)	C(79)-P(7)-C(85)-C(87)	51.08(16)
C(73)-Ir(4)-P(8)-C(89)	102.12(9)	C(81)-P(7)-C(85)-C(87)	162.21(14)
P(7)-Ir(4)-P(8)-C(89)	109.73(9)	Ir(4)-P(7)-C(85)-C(87)	-61.66(15)
N(7)-Ir(4)-C(73)-C(74)	-75(2)	C(80)-P(8)-C(89)-C(92)	165.84(14)
P(8)-Ir(4)-C(73)-C(74)	-173.90(15)	C(93)-P(8)-C(89)-C(92)	-83.33(16)
P(7)-Ir(4)-C(73)-C(74)	8.01(14)	Ir(4)-P(8)-C(89)-C(92)	52.74(15)
N(7)-Ir(4)-C(73)-C(78)	103(2)	C(80)-P(8)-C(89)-C(91)	-70.39(17)
P(8)-Ir(4)-C(73)-C(78)	4.33(15)	C(93)-P(8)-C(89)-C(91)	40.44(18)
P(7)-Ir(4)-C(73)-C(78)	-173.76(16)	Ir(4)-P(8)-C(89)-C(91)	176.51(13)
C(78)-C(73)-C(74)-C(75)	-0.3(3)	C(80)-P(8)-C(89)-C(90)	50.19(16)
Ir(4)-C(73)-C(74)-C(75)	178.06(15)	C(93)-P(8)-C(89)-C(90)	161.02(15)
C(78)-C(73)-C(74)-C(79)	-176.52(17)	Ir(4)-P(8)-C(89)-C(90)	-62.91(15)
Ir(4)-C(73)-C(74)-C(79)	1.8(2)	C(80)-P(8)-C(93)-C(95)	170.27(17)
C(73)-C(74)-C(75)-C(76)	-2.3(3)	C(89)-P(8)-C(93)-C(95)	58.16(19)
C(79)-C(74)-C(75)-C(76)	173.92(19)	Ir(4)-P(8)-C(93)-C(95)	-75.91(17)
C(74)-C(75)-C(76)-C(77)	2.3(3)	C(80)-P(8)-C(93)-C(94)	46.45(19)
C(75)-C(76)-C(77)-C(78)	0.4(3)	C(89)-P(8)-C(93)-C(94)	-65.66(19)
C(76)-C(77)-C(78)-C(73)	-3.1(3)	Ir(4)-P(8)-C(93)-C(94)	160.27(14)
C(76)-C(77)-C(78)-C(80)	174.3(2)	C(80)-P(8)-C(93)-C(96)	-72.77(19)
C(74)-C(73)-C(78)-C(77)	3.0(3)	C(89)-P(8)-C(93)-C(96)	175.12(17)
Ir(4)-C(73)-C(78)-C(77)	-175.37(15)	Ir(4)-P(8)-C(93)-C(96)	41.0(2)

Figure S-2 : ORTEP Diagram of complex 2

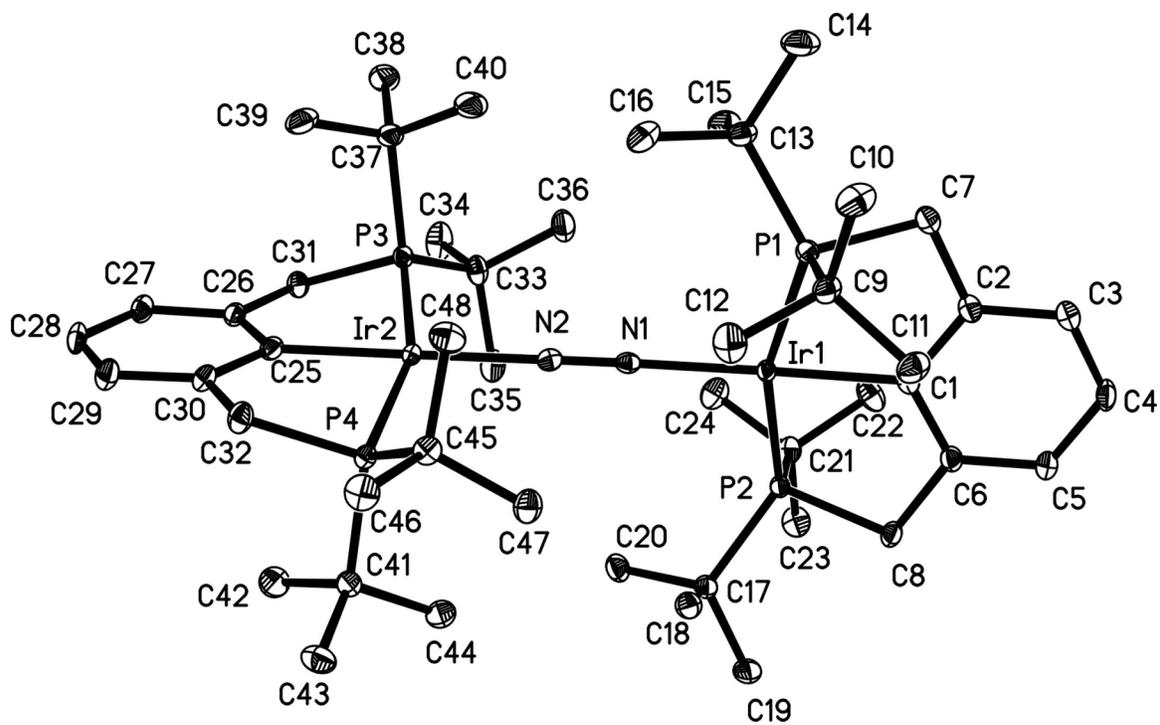


Table S-5. Crystal data and structure refinement for complex **2**.

Identification code	irhbzome	
Empirical formula	C ₅₁ H ₉₃ Ir ₂ N ₂ P ₄	
Formula weight	1242.55	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.2815(8) Å	α = 70.5540(10)°.
	b = 14.4823(8) Å	β = 89.0900(10)°.
	c = 14.7312(8) Å	γ = 69.7850(10)°.
Volume	2679.1(3) Å ³	
Z	2	
Density (calculated)	1.540 Mg/m ³	
Absorption coefficient	5.115 mm ⁻¹	
F(000)	1254	
Crystal size	0.42 x 0.33 x 0.22 mm ³	
Theta range for data collection	2.00 to 30.61°.	
Index ranges	-20 ≤ h ≤ 20, -20 ≤ k ≤ 20, -21 ≤ l ≤ 21	
Reflections collected	36737	
Independent reflections	16290 [R(int) = 0.0193]	
Completeness to theta = 30.61°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9999 and 0.6962	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	16290 / 0 / 557	
Goodness-of-fit on F ²	1.007	
Final R indices [I > 2σ(I)]	R1 = 0.0190, wR2 = 0.0459	
R indices (all data)	R1 = 0.0213, wR2 = 0.0468	
Largest diff. peak and hole	1.734 and -1.030 e.Å ⁻³	

Table S-6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for complex 2. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	7658(1)	2841(1)	4374(1)	9(1)
Ir(2)	5097(1)	2332(1)	2338(1)	9(1)
N(1)	6667(1)	2648(1)	3565(1)	11(1)
N(2)	6100(1)	2538(1)	3121(1)	11(1)
P(1)	8208(1)	3972(1)	3190(1)	11(1)
P(2)	7468(1)	1801(1)	5879(1)	10(1)
P(3)	6144(1)	886(1)	2026(1)	11(1)
P(4)	3675(1)	3711(1)	2327(1)	10(1)
C(1)	8657(1)	3041(1)	5211(1)	13(1)
C(2)	9403(1)	3444(2)	4818(1)	14(1)
C(3)	10080(2)	3580(2)	5391(1)	17(1)
C(4)	10050(2)	3302(2)	6388(1)	17(1)
C(5)	9327(2)	2902(2)	6803(1)	16(1)
C(6)	8643(1)	2782(1)	6228(1)	13(1)
C(7)	9446(1)	3752(2)	3741(1)	16(1)
C(8)	7861(2)	2359(2)	6689(1)	14(1)
C(9)	7483(2)	5412(2)	2950(1)	15(1)
C(10)	7836(2)	6165(2)	2143(2)	22(1)
C(11)	7586(2)	5625(2)	3892(1)	19(1)
C(12)	6372(2)	5634(2)	2710(2)	23(1)
C(13)	8505(2)	3733(2)	2021(1)	15(1)
C(14)	9270(2)	4190(2)	1492(2)	24(1)
C(15)	8972(2)	2532(2)	2309(2)	20(1)
C(16)	7544(2)	4133(2)	1334(1)	20(1)
C(17)	6167(1)	1899(2)	6197(1)	13(1)
C(18)	5499(1)	3052(2)	5665(1)	16(1)
C(19)	6056(2)	1645(2)	7288(1)	18(1)
C(20)	5798(2)	1202(2)	5823(1)	17(1)
C(21)	8364(1)	392(1)	6317(1)	14(1)
C(22)	9434(2)	410(2)	6365(2)	21(1)
C(23)	8205(2)	-285(2)	7314(1)	20(1)
C(24)	8281(2)	-96(2)	5560(2)	20(1)
C(25)	4084(1)	2114(1)	1537(1)	12(1)
C(26)	4282(1)	1155(1)	1373(1)	12(1)
C(27)	3601(2)	1008(2)	814(1)	15(1)
C(28)	2678(2)	1807(2)	408(1)	17(1)
C(29)	2454(2)	2750(2)	566(1)	17(1)
C(30)	3144(1)	2906(2)	1102(1)	14(1)
C(31)	5273(1)	281(1)	1812(1)	13(1)
C(32)	2898(2)	3945(1)	1238(1)	15(1)
C(33)	7086(1)	-233(1)	3011(1)	15(1)
C(34)	7339(2)	-1314(2)	2905(2)	25(1)
C(35)	6584(2)	-264(2)	3944(1)	19(1)
C(36)	8062(2)	-36(2)	3109(2)	22(1)
C(37)	6713(2)	1193(2)	853(1)	16(1)
C(38)	7399(2)	224(2)	647(2)	24(1)
C(39)	5855(2)	1818(2)	19(1)	21(1)
C(40)	7297(2)	1905(2)	865(2)	25(1)
C(41)	2862(1)	3412(2)	3324(1)	14(1)
C(42)	2511(2)	2553(2)	3231(2)	20(1)
C(43)	1937(2)	4350(2)	3315(2)	20(1)
C(44)	3513(2)	2956(2)	4297(1)	19(1)
C(45)	3771(1)	5027(1)	2096(1)	14(1)
C(46)	2782(2)	5970(2)	1662(2)	19(1)
C(47)	4170(2)	5080(2)	3030(1)	17(1)
C(48)	4534(2)	5119(2)	1354(2)	19(1)
C(49)	9882(2)	590(3)	9701(2)	44(1)
C(50)	10199(2)	1157(3)	10252(2)	47(1)
C(51)	9988(2)	2298(3)	9655(2)	46(1)

Table S-7. Bond lengths [Å] and angles [°] for complex 2.

Ir(1)-N(1)	2.0121(16)	C(17)-C(19)	1.543(3)
Ir(1)-C(1)	2.0534(18)	C(18)-H(18A)	0.9800
Ir(1)-P(1)	2.2989(5)	C(18)-H(18B)	0.9800
Ir(1)-P(2)	2.3028(5)	C(18)-H(18C)	0.9800
Ir(2)-N(2)	2.0115(16)	C(19)-H(19A)	0.9800
Ir(2)-C(25)	2.0511(18)	C(19)-H(19B)	0.9800
Ir(2)-P(3)	2.2985(5)	C(19)-H(19C)	0.9800
Ir(2)-P(4)	2.3001(5)	C(20)-H(20A)	0.9800
N(1)-N(2)	1.134(2)	C(20)-H(20B)	0.9800
P(1)-C(7)	1.8364(19)	C(20)-H(20C)	0.9800
P(1)-C(13)	1.8804(19)	C(21)-C(24)	1.530(3)
P(1)-C(9)	1.8902(19)	C(21)-C(23)	1.534(3)
P(2)-C(8)	1.8352(18)	C(21)-C(22)	1.541(3)
P(2)-C(17)	1.8768(19)	C(22)-H(22A)	0.9800
P(2)-C(21)	1.8873(19)	C(22)-H(22B)	0.9800
P(3)-C(31)	1.8345(18)	C(22)-H(22C)	0.9800
P(3)-C(33)	1.880(2)	C(23)-H(23A)	0.9800
P(3)-C(37)	1.8818(19)	C(23)-H(23B)	0.9800
P(4)-C(32)	1.8309(19)	C(23)-H(23C)	0.9800
P(4)-C(45)	1.8746(19)	C(24)-H(24A)	0.9800
P(4)-C(41)	1.8878(19)	C(24)-H(24B)	0.9800
C(1)-C(2)	1.414(3)	C(24)-H(24C)	0.9800
C(1)-C(6)	1.420(3)	C(25)-C(30)	1.415(3)
C(2)-C(3)	1.398(3)	C(25)-C(26)	1.420(2)
C(2)-C(7)	1.505(3)	C(26)-C(27)	1.398(2)
C(3)-C(4)	1.393(3)	C(26)-C(31)	1.506(3)
C(3)-H(3)	0.9500	C(27)-C(28)	1.394(3)
C(4)-C(5)	1.390(3)	C(27)-H(27)	0.9500
C(4)-H(4)	0.9500	C(28)-C(29)	1.389(3)
C(5)-C(6)	1.394(2)	C(28)-H(28)	0.9500
C(5)-H(5)	0.9500	C(29)-C(30)	1.393(3)
C(6)-C(8)	1.502(3)	C(29)-H(29)	0.9500
C(7)-H(7A)	0.9900	C(30)-C(32)	1.505(3)
C(7)-H(7B)	0.9900	C(31)-H(31A)	0.9900
C(8)-H(8A)	0.9900	C(31)-H(31B)	0.9900
C(8)-H(8B)	0.9900	C(32)-H(32A)	0.9900
C(9)-C(12)	1.529(3)	C(32)-H(32B)	0.9900
C(9)-C(10)	1.534(3)	C(33)-C(36)	1.533(3)
C(9)-C(11)	1.537(3)	C(33)-C(35)	1.534(3)
C(10)-H(10A)	0.9800	C(33)-C(34)	1.542(3)
C(10)-H(10B)	0.9800	C(34)-H(34A)	0.9800
C(10)-H(10C)	0.9800	C(34)-H(34B)	0.9800
C(11)-H(11A)	0.9800	C(34)-H(34C)	0.9800
C(11)-H(11B)	0.9800	C(35)-H(35A)	0.9800
C(11)-H(11C)	0.9800	C(35)-H(35B)	0.9800
C(12)-H(12A)	0.9800	C(35)-H(35C)	0.9800
C(12)-H(12B)	0.9800	C(36)-H(36A)	0.9800
C(12)-H(12C)	0.9800	C(36)-H(36B)	0.9800
C(13)-C(16)	1.533(3)	C(36)-H(36C)	0.9800
C(13)-C(15)	1.538(3)	C(37)-C(38)	1.531(3)
C(13)-C(14)	1.539(3)	C(37)-C(40)	1.537(3)
C(14)-H(14A)	0.9800	C(37)-C(39)	1.540(3)
C(14)-H(14B)	0.9800	C(38)-H(38A)	0.9800
C(14)-H(14C)	0.9800	C(38)-H(38B)	0.9800
C(15)-H(15A)	0.9800	C(38)-H(38C)	0.9800
C(15)-H(15B)	0.9800	C(39)-H(39A)	0.9800
C(15)-H(15C)	0.9800	C(39)-H(39B)	0.9800
C(16)-H(16A)	0.9800	C(39)-H(39C)	0.9800
C(16)-H(16B)	0.9800	C(40)-H(40A)	0.9800
C(16)-H(16C)	0.9800	C(40)-H(40B)	0.9800
C(17)-C(20)	1.532(3)	C(40)-H(40C)	0.9800
C(17)-C(18)	1.538(3)	C(41)-C(43)	1.529(3)

C(41)-C(44)	1.531(3)	C(47)-H(47A)	0.9800
C(41)-C(42)	1.538(3)	C(47)-H(47B)	0.9800
C(42)-H(42A)	0.9800	C(47)-H(47C)	0.9800
C(42)-H(42B)	0.9800	C(48)-H(48A)	0.9800
C(42)-H(42C)	0.9800	C(48)-H(48B)	0.9800
C(43)-H(43A)	0.9800	C(48)-H(48C)	0.9800
C(43)-H(43B)	0.9800	C(49)-C(50)	1.500(4)
C(43)-H(43C)	0.9800	C(49)-C(49)#1	1.556(7)
C(44)-H(44A)	0.9800	C(49)-H(49A)	0.9900
C(44)-H(44B)	0.9800	C(49)-H(49B)	0.9900
C(44)-H(44C)	0.9800	C(50)-C(51)	1.513(5)
C(45)-C(47)	1.533(3)	C(50)-H(50A)	0.9900
C(45)-C(48)	1.538(3)	C(50)-H(50B)	0.9900
C(45)-C(46)	1.543(3)	C(51)-H(51A)	0.9800
C(46)-H(46A)	0.9800	C(51)-H(51B)	0.9800
C(46)-H(46B)	0.9800	C(51)-H(51C)	0.9800
C(46)-H(46C)	0.9800		
N(1)-Ir(1)-C(1)	179.29(6)	C(2)-C(3)-H(3)	119.8
N(1)-Ir(1)-P(1)	100.35(4)	C(5)-C(4)-C(3)	118.98(17)
C(1)-Ir(1)-P(1)	80.15(5)	C(5)-C(4)-H(4)	120.5
N(1)-Ir(1)-P(2)	99.00(4)	C(3)-C(4)-H(4)	120.5
C(1)-Ir(1)-P(2)	80.49(5)	C(4)-C(5)-C(6)	120.43(18)
P(1)-Ir(1)-P(2)	160.630(16)	C(4)-C(5)-H(5)	119.8
N(2)-Ir(2)-C(25)	179.57(7)	C(6)-C(5)-H(5)	119.8
N(2)-Ir(2)-P(3)	99.07(4)	C(5)-C(6)-C(1)	122.44(17)
C(25)-Ir(2)-P(3)	80.50(5)	C(5)-C(6)-C(8)	119.61(16)
N(2)-Ir(2)-P(4)	100.28(4)	C(1)-C(6)-C(8)	117.95(15)
C(25)-Ir(2)-P(4)	80.14(5)	C(2)-C(7)-P(1)	107.07(13)
P(3)-Ir(2)-P(4)	160.623(16)	C(2)-C(7)-H(7A)	110.3
N(2)-N(1)-Ir(1)	178.97(15)	P(1)-C(7)-H(7A)	110.3
N(1)-N(2)-Ir(2)	179.64(16)	C(2)-C(7)-H(7B)	110.3
C(7)-P(1)-C(13)	102.51(9)	P(1)-C(7)-H(7B)	110.3
C(7)-P(1)-C(9)	103.61(9)	H(7A)-C(7)-H(7B)	108.6
C(13)-P(1)-C(9)	110.66(8)	C(6)-C(8)-P(2)	107.31(12)
C(7)-P(1)-Ir(1)	103.03(6)	C(6)-C(8)-H(8A)	110.3
C(13)-P(1)-Ir(1)	119.71(6)	P(2)-C(8)-H(8A)	110.3
C(9)-P(1)-Ir(1)	114.75(6)	C(6)-C(8)-H(8B)	110.3
C(8)-P(2)-C(17)	101.86(8)	P(2)-C(8)-H(8B)	110.3
C(8)-P(2)-C(21)	103.48(9)	H(8A)-C(8)-H(8B)	108.5
C(17)-P(2)-C(21)	111.36(8)	C(12)-C(9)-C(10)	109.89(17)
C(8)-P(2)-Ir(1)	102.54(6)	C(12)-C(9)-C(11)	107.35(16)
C(17)-P(2)-Ir(1)	118.87(6)	C(10)-C(9)-C(11)	108.29(15)
C(21)-P(2)-Ir(1)	115.84(6)	C(12)-C(9)-P(1)	108.37(13)
C(31)-P(3)-C(33)	101.92(8)	C(10)-C(9)-P(1)	114.61(14)
C(31)-P(3)-C(37)	103.51(8)	C(11)-C(9)-P(1)	108.07(13)
C(33)-P(3)-C(37)	110.75(9)	C(9)-C(10)-H(10A)	109.5
C(31)-P(3)-Ir(2)	102.68(6)	C(9)-C(10)-H(10B)	109.5
C(33)-P(3)-Ir(2)	120.41(6)	H(10A)-C(10)-H(10B)	109.5
C(37)-P(3)-Ir(2)	114.74(6)	C(9)-C(10)-H(10C)	109.5
C(32)-P(4)-C(45)	102.25(8)	H(10A)-C(10)-H(10C)	109.5
C(32)-P(4)-C(41)	103.09(9)	H(10B)-C(10)-H(10C)	109.5
C(45)-P(4)-C(41)	111.14(8)	C(9)-C(11)-H(11A)	109.5
C(32)-P(4)-Ir(2)	102.88(6)	C(9)-C(11)-H(11B)	109.5
C(45)-P(4)-Ir(2)	118.64(6)	H(11A)-C(11)-H(11B)	109.5
C(41)-P(4)-Ir(2)	116.03(6)	C(9)-C(11)-H(11C)	109.5
C(2)-C(1)-C(6)	115.38(16)	H(11A)-C(11)-H(11C)	109.5
C(2)-C(1)-Ir(1)	122.52(14)	H(11B)-C(11)-H(11C)	109.5
C(6)-C(1)-Ir(1)	122.10(13)	C(9)-C(12)-H(12A)	109.5
C(3)-C(2)-C(1)	122.28(17)	C(9)-C(12)-H(12B)	109.5
C(3)-C(2)-C(7)	119.70(17)	H(12A)-C(12)-H(12B)	109.5
C(1)-C(2)-C(7)	118.01(16)	C(9)-C(12)-H(12C)	109.5
C(4)-C(3)-C(2)	120.47(18)	H(12A)-C(12)-H(12C)	109.5
C(4)-C(3)-H(3)	119.8	H(12B)-C(12)-H(12C)	109.5

C(16)-C(13)-C(15)	108.47(16)	H(23A)-C(23)-H(23C)	109.5
C(16)-C(13)-C(14)	109.73(17)	H(23B)-C(23)-H(23C)	109.5
C(15)-C(13)-C(14)	107.55(17)	C(21)-C(24)-H(24A)	109.5
C(16)-C(13)-P(1)	110.81(13)	C(21)-C(24)-H(24B)	109.5
C(15)-C(13)-P(1)	105.12(13)	H(24A)-C(24)-H(24B)	109.5
C(14)-C(13)-P(1)	114.84(14)	C(21)-C(24)-H(24C)	109.5
C(13)-C(14)-H(14A)	109.5	H(24A)-C(24)-H(24C)	109.5
C(13)-C(14)-H(14B)	109.5	H(24B)-C(24)-H(24C)	109.5
H(14A)-C(14)-H(14B)	109.5	C(30)-C(25)-C(26)	115.19(16)
C(13)-C(14)-H(14C)	109.5	C(30)-C(25)-Ir(2)	122.68(13)
H(14A)-C(14)-H(14C)	109.5	C(26)-C(25)-Ir(2)	122.13(13)
H(14B)-C(14)-H(14C)	109.5	C(27)-C(26)-C(25)	122.35(17)
C(13)-C(15)-H(15A)	109.5	C(27)-C(26)-C(31)	119.76(16)
C(13)-C(15)-H(15B)	109.5	C(25)-C(26)-C(31)	117.88(16)
H(15A)-C(15)-H(15B)	109.5	C(28)-C(27)-C(26)	120.45(17)
C(13)-C(15)-H(15C)	109.5	C(28)-C(27)-H(27)	119.8
H(15A)-C(15)-H(15C)	109.5	C(26)-C(27)-H(27)	119.8
H(15B)-C(15)-H(15C)	109.5	C(29)-C(28)-C(27)	118.69(17)
C(13)-C(16)-H(16A)	109.5	C(29)-C(28)-H(28)	120.7
C(13)-C(16)-H(16B)	109.5	C(27)-C(28)-H(28)	120.7
H(16A)-C(16)-H(16B)	109.5	C(28)-C(29)-C(30)	120.83(18)
C(13)-C(16)-H(16C)	109.5	C(28)-C(29)-H(29)	119.6
H(16A)-C(16)-H(16C)	109.5	C(30)-C(29)-H(29)	119.6
H(16B)-C(16)-H(16C)	109.5	C(29)-C(30)-C(25)	122.44(17)
C(20)-C(17)-C(18)	108.52(15)	C(29)-C(30)-C(32)	119.97(17)
C(20)-C(17)-C(19)	109.61(15)	C(25)-C(30)-C(32)	117.59(16)
C(18)-C(17)-C(19)	107.82(15)	C(26)-C(31)-P(3)	107.14(12)
C(20)-C(17)-P(2)	110.93(13)	C(26)-C(31)-H(31A)	110.3
C(18)-C(17)-P(2)	105.36(12)	P(3)-C(31)-H(31A)	110.3
C(19)-C(17)-P(2)	114.33(13)	C(26)-C(31)-H(31B)	110.3
C(17)-C(18)-H(18A)	109.5	P(3)-C(31)-H(31B)	110.3
C(17)-C(18)-H(18B)	109.5	H(31A)-C(31)-H(31B)	108.5
H(18A)-C(18)-H(18B)	109.5	C(30)-C(32)-P(4)	107.24(12)
C(17)-C(18)-H(18C)	109.5	C(30)-C(32)-H(32A)	110.3
H(18A)-C(18)-H(18C)	109.5	P(4)-C(32)-H(32A)	110.3
H(18B)-C(18)-H(18C)	109.5	C(30)-C(32)-H(32B)	110.3
C(17)-C(19)-H(19A)	109.5	P(4)-C(32)-H(32B)	110.3
C(17)-C(19)-H(19B)	109.5	H(32A)-C(32)-H(32B)	108.5
H(19A)-C(19)-H(19B)	109.5	C(36)-C(33)-C(35)	108.64(16)
C(17)-C(19)-H(19C)	109.5	C(36)-C(33)-C(34)	109.18(17)
H(19A)-C(19)-H(19C)	109.5	C(35)-C(33)-C(34)	107.83(17)
H(19B)-C(19)-H(19C)	109.5	C(36)-C(33)-P(3)	111.79(14)
C(17)-C(20)-H(20A)	109.5	C(35)-C(33)-P(3)	104.71(13)
C(17)-C(20)-H(20B)	109.5	C(34)-C(33)-P(3)	114.41(14)
H(20A)-C(20)-H(20B)	109.5	C(33)-C(34)-H(34A)	109.5
C(17)-C(20)-H(20C)	109.5	C(33)-C(34)-H(34B)	109.5
H(20A)-C(20)-H(20C)	109.5	H(34A)-C(34)-H(34B)	109.5
H(20B)-C(20)-H(20C)	109.5	C(33)-C(34)-H(34C)	109.5
C(24)-C(21)-C(23)	110.02(16)	H(34A)-C(34)-H(34C)	109.5
C(24)-C(21)-C(22)	107.41(17)	H(34B)-C(34)-H(34C)	109.5
C(23)-C(21)-C(22)	108.82(16)	C(33)-C(35)-H(35A)	109.5
C(24)-C(21)-P(2)	108.65(13)	C(33)-C(35)-H(35B)	109.5
C(23)-C(21)-P(2)	114.52(14)	H(35A)-C(35)-H(35B)	109.5
C(22)-C(21)-P(2)	107.16(13)	C(33)-C(35)-H(35C)	109.5
C(21)-C(22)-H(22A)	109.5	H(35A)-C(35)-H(35C)	109.5
C(21)-C(22)-H(22B)	109.5	H(35B)-C(35)-H(35C)	109.5
H(22A)-C(22)-H(22B)	109.5	C(33)-C(36)-H(36A)	109.5
C(21)-C(22)-H(22C)	109.5	C(33)-C(36)-H(36B)	109.5
H(22A)-C(22)-H(22C)	109.5	H(36A)-C(36)-H(36B)	109.5
H(22B)-C(22)-H(22C)	109.5	C(33)-C(36)-H(36C)	109.5
C(21)-C(23)-H(23A)	109.5	H(36A)-C(36)-H(36C)	109.5
C(21)-C(23)-H(23B)	109.5	H(36B)-C(36)-H(36C)	109.5
H(23A)-C(23)-H(23B)	109.5	C(38)-C(37)-C(40)	110.07(17)
C(21)-C(23)-H(23C)	109.5	C(38)-C(37)-C(39)	108.02(16)

C(40)-C(37)-C(39)	107.68(18)	H(44A)-C(44)-H(44C)	109.5
C(38)-C(37)-P(3)	114.25(14)	H(44B)-C(44)-H(44C)	109.5
C(40)-C(37)-P(3)	108.34(13)	C(47)-C(45)-C(48)	109.03(16)
C(39)-C(37)-P(3)	108.27(13)	C(47)-C(45)-C(46)	109.18(15)
C(37)-C(38)-H(38A)	109.5	C(48)-C(45)-C(46)	107.71(16)
C(37)-C(38)-H(38B)	109.5	C(47)-C(45)-P(4)	110.35(13)
H(38A)-C(38)-H(38B)	109.5	C(48)-C(45)-P(4)	105.72(13)
C(37)-C(38)-H(38C)	109.5	C(46)-C(45)-P(4)	114.66(13)
H(38A)-C(38)-H(38C)	109.5	C(45)-C(46)-H(46A)	109.5
H(38B)-C(38)-H(38C)	109.5	C(45)-C(46)-H(46B)	109.5
C(37)-C(39)-H(39A)	109.5	H(46A)-C(46)-H(46B)	109.5
C(37)-C(39)-H(39B)	109.5	C(45)-C(46)-H(46C)	109.5
H(39A)-C(39)-H(39B)	109.5	H(46A)-C(46)-H(46C)	109.5
C(37)-C(39)-H(39C)	109.5	H(46B)-C(46)-H(46C)	109.5
H(39A)-C(39)-H(39C)	109.5	C(45)-C(47)-H(47A)	109.5
H(39B)-C(39)-H(39C)	109.5	C(45)-C(47)-H(47B)	109.5
C(37)-C(40)-H(40A)	109.5	H(47A)-C(47)-H(47B)	109.5
C(37)-C(40)-H(40B)	109.5	C(45)-C(47)-H(47C)	109.5
H(40A)-C(40)-H(40B)	109.5	H(47A)-C(47)-H(47C)	109.5
C(37)-C(40)-H(40C)	109.5	H(47B)-C(47)-H(47C)	109.5
H(40A)-C(40)-H(40C)	109.5	C(45)-C(48)-H(48A)	109.5
H(40B)-C(40)-H(40C)	109.5	C(45)-C(48)-H(48B)	109.5
C(43)-C(41)-C(44)	109.58(16)	H(48A)-C(48)-H(48B)	109.5
C(43)-C(41)-C(42)	108.53(16)	C(45)-C(48)-H(48C)	109.5
C(44)-C(41)-C(42)	107.35(16)	H(48A)-C(48)-H(48C)	109.5
C(43)-C(41)-P(4)	114.92(13)	H(48B)-C(48)-H(48C)	109.5
C(44)-C(41)-P(4)	108.23(13)	C(50)-C(49)-C(49)#1	113.1(3)
C(42)-C(41)-P(4)	107.97(13)	C(50)-C(49)-H(49A)	109.0
C(41)-C(42)-H(42A)	109.5	C(49)#1-C(49)-H(49A)	109.0
C(41)-C(42)-H(42B)	109.5	C(50)-C(49)-H(49B)	109.0
H(42A)-C(42)-H(42B)	109.5	C(49)#1-C(49)-H(49B)	109.0
C(41)-C(42)-H(42C)	109.5	H(49A)-C(49)-H(49B)	107.8
H(42A)-C(42)-H(42C)	109.5	C(49)-C(50)-C(51)	112.6(3)
H(42B)-C(42)-H(42C)	109.5	C(49)-C(50)-H(50A)	109.1
C(41)-C(43)-H(43A)	109.5	C(51)-C(50)-H(50A)	109.1
C(41)-C(43)-H(43B)	109.5	C(49)-C(50)-H(50B)	109.1
H(43A)-C(43)-H(43B)	109.5	C(51)-C(50)-H(50B)	109.1
C(41)-C(43)-H(43C)	109.5	H(50A)-C(50)-H(50B)	107.8
H(43A)-C(43)-H(43C)	109.5	C(50)-C(51)-H(51A)	109.5
H(43B)-C(43)-H(43C)	109.5	C(50)-C(51)-H(51B)	109.5
C(41)-C(44)-H(44A)	109.5	H(51A)-C(51)-H(51B)	109.5
C(41)-C(44)-H(44B)	109.5	C(50)-C(51)-H(51C)	109.5
H(44A)-C(44)-H(44B)	109.5	H(51A)-C(51)-H(51C)	109.5
C(41)-C(44)-H(44C)	109.5	H(51B)-C(51)-H(51C)	109.5

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y,-z+2

Table S-8. Torsion angles [°] for complex 2.

C(1)-Ir(1)-N(1)-N(2)	-12(12)	Ir(1)-C(1)-C(6)-C(8)	-0.5(2)
P(1)-Ir(1)-N(1)-N(2)	-147(8)	C(3)-C(2)-C(7)-P(1)	-157.69(16)
P(2)-Ir(1)-N(1)-N(2)	32(8)	C(1)-C(2)-C(7)-P(1)	21.2(2)
Ir(1)-N(1)-N(2)-Ir(2)	-74(30)	C(13)-P(1)-C(7)-C(2)	-155.14(13)
C(25)-Ir(2)-N(2)-N(1)	-53(29)	C(9)-P(1)-C(7)-C(2)	89.67(14)
P(3)-Ir(2)-N(2)-N(1)	-47(26)	Ir(1)-P(1)-C(7)-C(2)	-30.21(14)
P(4)-Ir(2)-N(2)-N(1)	133(26)	C(5)-C(6)-C(8)-P(2)	-156.83(15)
N(1)-Ir(1)-P(1)-C(7)	-156.45(8)	C(1)-C(6)-C(8)-P(2)	22.8(2)
C(1)-Ir(1)-P(1)-C(7)	24.06(8)	C(17)-P(2)-C(8)-C(6)	-154.61(13)
P(2)-Ir(1)-P(1)-C(7)	26.31(9)	C(21)-P(2)-C(8)-C(6)	89.72(14)
N(1)-Ir(1)-P(1)-C(13)	-43.61(9)	Ir(1)-P(2)-C(8)-C(6)	-31.11(13)
C(1)-Ir(1)-P(1)-C(13)	136.90(9)	C(7)-P(1)-C(9)-C(12)	-167.04(13)
P(2)-Ir(1)-P(1)-C(13)	139.15(8)	C(13)-P(1)-C(9)-C(12)	83.71(15)
N(1)-Ir(1)-P(1)-C(9)	91.67(8)	Ir(1)-P(1)-C(9)-C(12)	-55.51(14)
C(1)-Ir(1)-P(1)-C(9)	-87.82(8)	C(7)-P(1)-C(9)-C(10)	69.83(16)
P(2)-Ir(1)-P(1)-C(9)	-85.57(8)	C(13)-P(1)-C(9)-C(10)	-39.41(17)
N(1)-Ir(1)-P(2)-C(8)	-155.29(8)	Ir(1)-P(1)-C(9)-C(10)	-178.63(12)
C(1)-Ir(1)-P(2)-C(8)	24.21(8)	C(7)-P(1)-C(9)-C(11)	-51.01(15)
P(1)-Ir(1)-P(2)-C(8)	21.96(9)	C(13)-P(1)-C(9)-C(11)	-160.25(13)
N(1)-Ir(1)-P(2)-C(17)	-44.01(8)	Ir(1)-P(1)-C(9)-C(11)	60.53(14)
C(1)-Ir(1)-P(2)-C(17)	135.49(9)	C(7)-P(1)-C(13)-C(16)	-166.24(14)
P(1)-Ir(1)-P(2)-C(17)	133.25(8)	C(9)-P(1)-C(13)-C(16)	-56.28(15)
N(1)-Ir(1)-P(2)-C(21)	92.80(8)	Ir(1)-P(1)-C(13)-C(16)	80.64(14)
C(1)-Ir(1)-P(2)-C(21)	-87.70(8)	C(7)-P(1)-C(13)-C(15)	76.78(14)
P(1)-Ir(1)-P(2)-C(21)	-89.94(8)	C(9)-P(1)-C(13)-C(15)	-173.27(13)
N(2)-Ir(2)-P(3)-C(31)	155.62(7)	Ir(1)-P(1)-C(13)-C(15)	-36.34(15)
C(25)-Ir(2)-P(3)-C(31)	-24.42(8)	C(7)-P(1)-C(13)-C(14)	-41.21(17)
P(4)-Ir(2)-P(3)-C(31)	-27.04(8)	C(9)-P(1)-C(13)-C(14)	68.74(17)
N(2)-Ir(2)-P(3)-C(33)	43.44(8)	Ir(1)-P(1)-C(13)-C(14)	-154.33(13)
C(25)-Ir(2)-P(3)-C(33)	-136.60(9)	C(8)-P(2)-C(17)-C(20)	-163.95(13)
P(4)-Ir(2)-P(3)-C(33)	-139.22(8)	C(21)-P(2)-C(17)-C(20)	-54.20(15)
N(2)-Ir(2)-P(3)-C(37)	-92.84(8)	Ir(1)-P(2)-C(17)-C(20)	84.39(13)
C(25)-Ir(2)-P(3)-C(37)	87.12(9)	C(8)-P(2)-C(17)-C(18)	78.81(13)
P(4)-Ir(2)-P(3)-C(37)	84.50(8)	C(21)-P(2)-C(17)-C(18)	-171.44(11)
N(2)-Ir(2)-P(4)-C(32)	155.86(8)	Ir(1)-P(2)-C(17)-C(18)	-32.85(14)
C(25)-Ir(2)-P(4)-C(32)	-24.10(8)	C(8)-P(2)-C(17)-C(19)	-39.39(16)
P(3)-Ir(2)-P(4)-C(32)	-21.47(9)	C(21)-P(2)-C(17)-C(19)	70.36(15)
N(2)-Ir(2)-P(4)-C(45)	43.97(8)	Ir(1)-P(2)-C(17)-C(19)	-151.05(12)
C(25)-Ir(2)-P(4)-C(45)	-135.98(8)	C(8)-P(2)-C(21)-C(24)	-166.88(14)
P(3)-Ir(2)-P(4)-C(45)	-133.36(8)	C(17)-P(2)-C(21)-C(24)	84.41(15)
N(2)-Ir(2)-P(4)-C(41)	-92.42(8)	Ir(1)-P(2)-C(21)-C(24)	-55.53(15)
C(25)-Ir(2)-P(4)-C(41)	87.63(8)	C(8)-P(2)-C(21)-C(23)	69.68(15)
P(3)-Ir(2)-P(4)-C(41)	90.25(8)	C(17)-P(2)-C(21)-C(23)	-39.03(16)
N(1)-Ir(1)-C(1)-C(2)	-153(5)	Ir(1)-P(2)-C(21)-C(23)	-178.97(12)
P(1)-Ir(1)-C(1)-C(2)	-17.47(14)	C(8)-P(2)-C(21)-C(22)	-51.11(15)
P(2)-Ir(1)-C(1)-C(2)	163.28(16)	C(17)-P(2)-C(21)-C(22)	-159.82(13)
N(1)-Ir(1)-C(1)-C(6)	27(5)	Ir(1)-P(2)-C(21)-C(22)	60.24(14)
P(1)-Ir(1)-C(1)-C(6)	162.48(16)	N(2)-Ir(2)-C(25)-C(30)	-157(9)
P(2)-Ir(1)-C(1)-C(6)	-16.77(14)	P(3)-Ir(2)-C(25)-C(30)	-162.31(15)
C(6)-C(1)-C(2)-C(3)	-0.1(3)	P(4)-Ir(2)-C(25)-C(30)	16.81(14)
Ir(1)-C(1)-C(2)-C(3)	179.88(15)	N(2)-Ir(2)-C(25)-C(26)	22(10)
C(6)-C(1)-C(2)-C(7)	-178.96(17)	P(3)-Ir(2)-C(25)-C(26)	17.07(14)
Ir(1)-C(1)-C(2)-C(7)	1.0(2)	P(4)-Ir(2)-C(25)-C(26)	-163.81(15)
C(1)-C(2)-C(3)-C(4)	1.0(3)	C(30)-C(25)-C(26)-C(27)	0.6(3)
C(7)-C(2)-C(3)-C(4)	179.90(19)	Ir(2)-C(25)-C(26)-C(27)	-178.85(14)
C(2)-C(3)-C(4)-C(5)	-1.0(3)	C(30)-C(25)-C(26)-C(31)	179.61(16)
C(3)-C(4)-C(5)-C(6)	0.0(3)	Ir(2)-C(25)-C(26)-C(31)	0.2(2)
C(4)-C(5)-C(6)-C(1)	1.0(3)	C(25)-C(26)-C(27)-C(28)	-1.3(3)
C(4)-C(5)-C(6)-C(8)	-179.34(18)	C(31)-C(26)-C(27)-C(28)	179.64(17)
C(2)-C(1)-C(6)-C(5)	-1.0(3)	C(26)-C(27)-C(28)-C(29)	0.3(3)
Ir(1)-C(1)-C(6)-C(5)	179.10(14)	C(27)-C(28)-C(29)-C(30)	1.4(3)
C(2)-C(1)-C(6)-C(8)	179.41(17)	C(28)-C(29)-C(30)-C(25)	-2.2(3)

C(28)-C(29)-C(30)-C(32)	178.12(18)	Ir(2)-P(3)-C(37)-C(38)	-179.33(12)
C(26)-C(25)-C(30)-C(29)	1.2(3)	C(31)-P(3)-C(37)-C(40)	168.64(15)
Ir(2)-C(25)-C(30)-C(29)	-179.40(15)	C(33)-P(3)-C(37)-C(40)	-82.81(16)
C(26)-C(25)-C(30)-C(32)	-179.13(16)	Ir(2)-P(3)-C(37)-C(40)	57.59(16)
Ir(2)-C(25)-C(30)-C(32)	0.3(2)	C(31)-P(3)-C(37)-C(39)	52.13(15)
C(27)-C(26)-C(31)-P(3)	156.46(15)	C(33)-P(3)-C(37)-C(39)	160.68(13)
C(25)-C(26)-C(31)-P(3)	-22.6(2)	Ir(2)-P(3)-C(37)-C(39)	-58.92(14)
C(33)-P(3)-C(31)-C(26)	156.44(12)	C(32)-P(4)-C(41)-C(43)	-69.99(15)
C(37)-P(3)-C(31)-C(26)	-88.53(13)	C(45)-P(4)-C(41)-C(43)	38.87(16)
Ir(2)-P(3)-C(31)-C(26)	31.15(13)	Ir(2)-P(4)-C(41)-C(43)	178.40(12)
C(29)-C(30)-C(32)-P(4)	157.23(15)	C(32)-P(4)-C(41)-C(44)	167.18(13)
C(25)-C(30)-C(32)-P(4)	-22.5(2)	C(45)-P(4)-C(41)-C(44)	-83.95(15)
C(45)-P(4)-C(32)-C(30)	154.46(13)	Ir(2)-P(4)-C(41)-C(44)	55.58(14)
C(41)-P(4)-C(32)-C(30)	-90.11(14)	C(32)-P(4)-C(41)-C(42)	51.27(15)
Ir(2)-P(4)-C(32)-C(30)	30.91(14)	C(45)-P(4)-C(41)-C(42)	160.14(13)
C(31)-P(3)-C(33)-C(36)	162.60(14)	Ir(2)-P(4)-C(41)-C(42)	-60.33(14)
C(37)-P(3)-C(33)-C(36)	53.01(16)	C(32)-P(4)-C(45)-C(47)	165.84(13)
Ir(2)-P(3)-C(33)-C(36)	-84.82(14)	C(41)-P(4)-C(45)-C(47)	56.43(15)
C(31)-P(3)-C(33)-C(35)	-79.97(13)	Ir(2)-P(4)-C(45)-C(47)	-81.92(14)
C(37)-P(3)-C(33)-C(35)	170.44(12)	C(32)-P(4)-C(45)-C(48)	-76.40(14)
Ir(2)-P(3)-C(33)-C(35)	32.61(14)	C(41)-P(4)-C(45)-C(48)	174.18(12)
C(31)-P(3)-C(33)-C(34)	37.86(17)	Ir(2)-P(4)-C(45)-C(48)	35.83(14)
C(37)-P(3)-C(33)-C(34)	-71.73(17)	C(32)-P(4)-C(45)-C(46)	42.08(16)
Ir(2)-P(3)-C(33)-C(34)	150.43(13)	C(41)-P(4)-C(45)-C(46)	-67.34(15)
C(31)-P(3)-C(37)-C(38)	-68.28(16)	Ir(2)-P(4)-C(45)-C(46)	154.31(11)
C(33)-P(3)-C(37)-C(38)	40.28(16)	C(49)#1-C(49)-C(50)-C(51)	178.7(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y,-z+2