8 Appendix

8.1 Crystal data for 124

Table 1. Crystal data and structure refinement for 2011ncs0393a.

Identification code	2011ncs0393a	
Empirical formula	C41 H51 F6 Ir N2 P2	
Formula weight	939.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8078(4) Å	α= 81.857(6)°.
	b = 11.5085(5) Å	β= 74.350(5)°.
	c = 16.2964(11) Å	γ = 77.326(6)°.
Volume	1896.92(17) $Å^3$	
Z	2	
Density (calculated)	1.646 Mg/m^3	
Absorption coefficient	3.666 mm^{-1}	
F(000)	944	
Crystal size	0.04 x 0.03 x 0.02 mm^3	
Theta range for data collection	3.71 to 27.48°.	
Index ranges	-13<=h<=14, -14<=k<=14, -21<=l<=21	
Reflections collected	41255	
Independent reflections	8661 [R(int) = 0.0790]	
Completeness to theta = 27.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.681	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8661 / 0 / 469	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.0862	
R indices (all data)	R1 = 0.0493, wR2 = 0.0901	
Largest diff. peak and hole	1.191 and -1.850 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2011ncs0393a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	3276(1)	8029(1)	1727(1)	23(1)
P(1)	2665(1)	7267(1)	3137(1)	23(1)
P(2)	8811(1)	1449(1)	1999(1)	32(1)
F(1)	8892(3)	420(3)	1406(2)	49(1)
F(2)	8775(3)	2437(3)	2594(2)	42(1)
F(3)	7490(3)	2127(3)	1770(2)	45(1)
F(4)	9665(3)	2104(3)	1201(2)	49(1)
F(5)	8013(3)	708(3)	2786(2)	50(1)
F(6)	10148(3)	711(3)	2231(2)	51(1)
N(1)	4446(3)	9924(3)	2243(2)	25(1)
N(2)	5944(3)	8382(3)	1906(2)	25(1)
C(1)	4287(4)	7989(4)	374(2)	27(1)
C(2)	3989(5)	7025(4)	-52(3)	37(1)
C(3)	3183(5)	6189(4)	577(3)	36(1)
C(4)	2293(4)	6759(4)	1361(3)	30(1)
C(5)	1364(5)	8611(4)	522(3)	35(1)
C(6)	2234(5)	9548(4)	278(3)	34(1)
C(7)	3527(4)	9112(4)	485(3)	28(1)
C(8)	1506(4)	7872(4)	1347(3)	30(1)
C(9)	4648(4)	8800(4)	1985(2)	22(1)
C(10)	5599(4)	10162(4)	2342(3)	28(1)
C(11)	6523(4)	9196(4)	2133(3)	28(1)
C(12)	3209(4)	10810(4)	2368(3)	24(1)
C(13)	3386(4)	11877(4)	1701(3)	30(1)
C(14)	2142(4)	12843(4)	1812(3)	36(1)
C(15)	1700(5)	13231(4)	2712(3)	41(1)
C(16)	1534(4)	12160(4)	3378(3)	35(1)
C(17)	2785(4)	11214(4)	3272(3)	30(1)
C(18)	6682(4)	7188(4)	1644(3)	27(1)
C(19)	7801(4)	7338(4)	859(3)	32(1)
C(20)	8661(5)	6129(5)	607(3)	41(1)
C(21)	9179(5)	5456(5)	1352(3)	43(1)
C(22)	8051(5)	5269(4)	2117(3)	36(1)
C(23)	7195(4)	6454(4)	2383(3)	30(1)
C(24)	971(4)	7063(4)	3515(3)	25(1)
C(25)	-15(4)	8062(4)	3480(3)	29(1)
C(26)	-1319(4)	7969(5)	3798(3)	34(1)
C(27)	-1654(4)	6869(5)	4133(3)	35(1)
C(28)	-687(4)	5872(5)	4156(3)	34(1)
C(29)	634(4)	5956(4)	3848(3)	29(1)
C(30)	2871(4)	8019(4)	3998(3)	25(1)
C(31)	4127(4)	8166(4)	3975(3)	28(1)
C(32)	4356(5)	8689(4)	4619(3)	31(1)
C(33)	3320(5)	9089(4)	5299(3)	32(1)
C(34)	2076(5)	8958(4)	5331(3)	35(1)
C(35)	1852(4)	8420(4)	4679(3)	30(1)

C(36)	3659(4)	5780(4)	3298(3)	26(1)
C(37)	4334(4)	5153(4)	2593(3)	29(1)
C(38)	5142(4)	4048(4)	2693(3)	33(1)
C(39)	5276(5)	3574(4)	3494(3)	36(1)
C(40)	4600(5)	4193(4)	4204(3)	37(1)
C(41)	3787(4)	5284(4)	4110(3)	30(1)

Table 3. Bond lengths [Å] and angles [°] for 2011ncs0393a.

Ir(1)-C(9)	2.045(4)
Ir(1)-C(1)	2.183(4)
Ir(1)-C(7)	2.205(4)
Ir(1)-C(4)	2.212(4)
Ir(1)-C(8)	2.214(4)
Ir(1)-P(1)	2.3131(11)
P(1)-C(24)	1.824(4)
P(1)-C(36)	1.835(4)
P(1)-C(30)	1.835(4)
P(2)-F(4)	1.579(3)
P(2)-F(3)	1.583(3)
P(2)-F(2)	1.583(3)
P(2)-F(5)	1.591(3)
P(2)-F(1)	1.605(3)
P(2)-F(6)	1.618(3)
N(1)-C(9)	1.370(5)
N(1)-C(10)	1.388(5)
N(1)-C(12)	1.477(5)
N(2)-C(9)	1.354(5)
N(2)-C(11)	1.374(5)
N(2)-C(18)	1.487(5)
C(1)-C(7)	1.378(6)
C(1)-C(2)	1.520(6)
C(1)-H(1)	0.9500
C(2)-C(3)	1.530(6)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.512(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(8)	1.375(6)
C(4)-H(4)	0.9500
C(5)-C(8)	1.511(6)
C(5)-C(6)	1.525(7)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.489(6)
C(6)-H(6A)	0.9900

C(6)-H(6B)	0.9900
C(7)-H(7)	0.9500
C(8)-H(8)	0.9500
C(10)-C(11)	1.336(6)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(17)	1.527(6)
C(12)-C(13)	1.530(6)
C(12)-H(12)	1.0000
C(13)-C(14)	1.531(6)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.514(7)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.530(7)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.525(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.524(6)
C(18)-C(23)	1.530(6)
C(18)-H(18)	1.0000
C(19)-C(20)	1.536(6)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.514(8)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.519(7)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.517(6)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.392(6)
C(24)-C(29)	1.397(6)
C(25)-C(26)	1.386(6)
C(25)-H(25)	0.9500
C(26)-C(27)	1.390(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.376(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.400(6)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-C(35)	1.385(6)

C(30)-C(31)	1.393(6)
C(31)-C(32)	1.382(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.394(6)
C(32)-H(32)	0.9500
C(33)-C(34)	1.372(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.400(6)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-C(37)	1.388(6)
C(36)-C(41)	1.395(6)
C(37)-C(38)	1.392(6)
C(37)-H(37)	0.9500
C(38)-C(39)	1.374(7)
C(38)-H(38)	0.9500
C(39)-C(40)	1.389(7)
C(39)-H(39)	0.9500
C(40)-C(41)	1.381(6)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500

C(9)-Ir(1)-C(1)	92.41(16)
C(9)-Ir(1)-C(7)	88.02(16)
C(1)-Ir(1)-C(7)	36.60(16)
C(9)-Ir(1)-C(4)	163.05(17)
C(1)-Ir(1)-C(4)	80.46(16)
C(7)-Ir(1)-C(4)	95.04(17)
C(9)-Ir(1)-C(8)	159.59(17)
C(1)-Ir(1)-C(8)	86.73(16)
C(7)-Ir(1)-C(8)	79.15(17)
C(4)-Ir(1)-C(8)	36.19(17)
C(9)-Ir(1)-P(1)	91.54(11)
C(1)-Ir(1)-P(1)	156.25(13)
C(7)-Ir(1)-P(1)	167.08(12)
C(4)-Ir(1)-P(1)	89.14(12)
C(8)-Ir(1)-P(1)	97.44(12)
C(24)-P(1)-C(36)	105.3(2)
C(24)-P(1)-C(30)	102.66(19)
C(36)-P(1)-C(30)	101.0(2)
C(24)-P(1)-Ir(1)	115.54(15)
C(36)-P(1)-Ir(1)	110.18(14)
C(30)-P(1)-Ir(1)	120.35(14)
F(4)-P(2)-F(3)	92.21(18)
F(4)-P(2)-F(2)	91.56(17)
F(3)-P(2)-F(2)	92.40(16)
F(4)-P(2)-F(5)	176.2(2)
F(3)-P(2)-F(5)	90.32(18)
F(2)-P(2)-F(5)	91.15(17)
F(4)-P(2)-F(1)	88.54(17)
F(3)-P(2)-F(1)	89.61(17)
F(2)-P(2)-F(1)	177.98(19)

F(5)-P(2)-F(1)	88.66(17)
F(4)-P(2)-F(6)	88.81(17)
F(3)-P(2)-F(6)	177.97(18)
F(2)-P(2)-F(6)	89.33(16)
F(5)-P(2)-F(6)	88.58(18)
F(1)-P(2)-F(6)	88.66(17)
C(9)-N(1)-C(10)	110.6(3)
C(9)-N(1)-C(12)	126.4(4)
C(10)-N(1)-C(12)	122.9(4)
C(9)-N(2)-C(11)	111.3(4)
C(9)-N(2)-C(18)	126.3(4)
C(11)-N(2)-C(18)	122.4(4)
C(7)-C(1)-C(2)	125.0(4)
C(7)-C(1)-Ir(1)	72.6(2)
C(2)-C(1)-Ir(1)	113.2(3)
C(7)-C(1)-H(1)	117.5
C(2)-C(1)-H(1)	117.5
Ir(1)-C(1)-H(1)	84.1
C(1)-C(2)-C(3)	113.4(4)
C(1)-C(2)-H(2A)	108.9
C(3)-C(2)-H(2A)	108.9
C(1)-C(2)-H(2B)	108.9
C(3)-C(2)-H(2B)	108.9
H(2A)-C(2)-H(2B)	107.7
C(4)-C(3)-C(2)	114.3(4)
C(4)-C(3)-H(3A)	108.7
C(2)-C(3)-H(3A)	108.7
C(4)-C(3)-H(3B)	108.7
C(2)-C(3)-H(3B)	108.7
H(3A)-C(3)-H(3B)	107.6
C(8)-C(4)-C(3)	124.5(4)
C(8)-C(4)-Ir(1)	72.0(3)
C(3)-C(4)-Ir(1)	108.7(3)
C(8)-C(4)-H(4)	117.7
C(3)-C(4)-H(4)	117.7
Ir(1)-C(4)-H(4)	89.3
C(8)-C(5)-C(6)	112.2(4)
C(8)-C(5)-H(5A)	109.2
C(6)-C(5)-H(5A)	109.2
C(8)-C(5)-H(5B)	109.2
C(6)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9
C(7)-C(6)-C(5)	112.8(4)
C(7)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6A)	109.0
C(7)-C(6)-H(6B)	109.0
C(5)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(1)-C(7)-C(6)	126.0(4)
C(1)-C(7)-Ir(1)	70.8(2)
C(6)-C(7)-Ir(1)	109.8(3)
C(1)-C(7)-H(7)	117.0

C(6)-C(7)-H(7)	117.0
Ir(1)-C(7)-H(7)	89.3
C(4)-C(8)-C(5)	122.4(4)
C(4)-C(8)-Ir(1)	71.8(3)
C(5)-C(8)-Ir(1)	112.8(3)
C(4)-C(8)-H(8)	118.8
C(5)-C(8)-H(8)	118.8
Ir(1)-C(8)-H(8)	85.4
N(2)-C(9)-N(1)	103.9(3)
N(2)-C(9)-Ir(1)	129.8(3)
N(1)-C(9)-Ir(1)	126.1(3)
C(11)-C(10)-N(1)	106.7(4)
C(11)-C(10)-H(10)	126.7
N(1)-C(10)-H(10)	126.7
C(10)-C(11)-N(2)	107.5(4)
C(10)-C(11)-H(11)	126.3
N(2)-C(11)-H(11)	126.3
N(1)-C(12)-C(17)	111.2(3)
N(1)-C(12)-C(13)	109.1(3)
C(17)-C(12)-C(13)	110.7(4)
N(1)-C(12)-H(12)	108.6
C(17)-C(12)-H(12)	108.6
C(13)-C(12)-H(12)	108.6
C(12)-C(13)-C(14)	111.5(4)
C(12)-C(13)-H(13A)	109.3
C(14)-C(13)-H(13A)	109.3
C(12)-C(13)-H(13B)	109.3
C(14)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	108.0
C(15)-C(14)-C(13)	111.3(4)
C(15)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14B)	109.4
C(13)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
C(14)-C(15)-C(16)	111.3(4)
C(14)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15B)	109.4
C(16)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(17)-C(16)-C(15)	111.5(4)
C(17)-C(16)-H(16A)	109.3
C(15)-C(16)-H(16A)	109.3
C(17)-C(16)-H(16B)	109.3
C(15)-C(16)-H(16B)	109.3
H(16A)-C(16)-H(16B)	108.0
C(16)-C(17)-C(12)	110.5(4)
C(16)-C(17)-H(17A)	109.6
C(12)-C(17)-H(17A)	109.6
C(16)-C(17)-H(17B)	109.6
C(12)-C(17)-H(17B)	109.6

H(17A)-C(17)-H(17B)	108.1
N(2)-C(18)-C(19)	109.7(3)
N(2)-C(18)-C(23)	110.2(3)
C(19)-C(18)-C(23)	111.0(4)
N(2)-C(18)-H(18)	108.7
C(19)-C(18)-H(18)	108.7
C(23)-C(18)-H(18)	108.7
C(18)-C(19)-C(20)	111.6(4)
C(18)-C(19)-H(19A)	109.3
C(20)-C(19)-H(19A)	109.3
C(18)-C(19)-H(19B)	109.3
C(20)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	108.0
C(21)-C(20)-C(19)	110.6(4)
C(21)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20A)	109.5
C(21)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	108.1
C(20)-C(21)-C(22)	110.2(4)
C(20)-C(21)-H(21A)	109.6
C(22)-C(21)-H(21A)	109.6
C(20)-C(21)-H(21B)	109.6
C(22)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1
C(23)-C(22)-C(21)	111.1(4)
C(23)-C(22)-H(22A)	109.4
C(21)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22B)	109.4
C(21)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
C(22)-C(23)-C(18)	111.7(4)
C(22)-C(23)-H(23A)	109.3
C(18)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23B)	109.3
C(18)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	107.9
C(25)-C(24)-C(29)	119.4(4)
C(25)-C(24)-P(1)	118.1(3)
C(29)-C(24)-P(1)	122.6(3)
C(26)-C(25)-C(24)	120.4(4)
C(26)-C(25)-H(25)	119.8
C(24)-C(25)-H(25)	119.8
C(25)-C(26)-C(27)	120.2(4)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(28)-C(27)-C(26)	119.8(4)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(27)-C(28)-C(29)	120.6(4)
C(27)-C(28)-H(28)	119.7
C(29)-C(28)-H(28)	119.7

C(24)-C(29)-C(28)	119.6(4)
C(24)-C(29)-H(29)	120.2
C(28)-C(29)-H(29)	120.2
C(35)-C(30)-C(31)	118.5(4)
C(35)-C(30)-P(1)	123.4(3)
C(31)-C(30)-P(1)	118.0(3)
C(32)-C(31)-C(30)	120.9(4)
C(32)-C(31)-H(31)	119.5
C(30)-C(31)-H(31)	119.5
C(31)-C(32)-C(33)	119.9(4)
C(31)-C(32)-H(32)	120.1
C(33)-C(32)-H(32)	120.1
C(34)-C(33)-C(32)	120.0(4)
C(34)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(33)-C(34)-C(35)	119.8(4)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(30)-C(35)-C(34)	120.8(4)
C(30)-C(35)-H(35)	119.6
C(34)-C(35)-H(35)	119.6
C(37)-C(36)-C(41)	119.2(4)
C(37)-C(36)-P(1)	119.3(4)
C(41)-C(36)-P(1)	121.5(3)
C(36)-C(37)-C(38)	120.5(4)
C(36)-C(37)-H(37)	119.8
C(38)-C(37)-H(37)	119.8
C(39)-C(38)-C(37)	119.9(4)
C(39)-C(38)-H(38)	120.1
C(37)-C(38)-H(38)	120.1
C(38)-C(39)-C(40)	120.1(5)
C(38)-C(39)-H(39)	119.9
C(40)-C(39)-H(39)	119.9
C(41)-C(40)-C(39)	120.2(5)
C(41)-C(40)-H(40)	119.9
C(39)-C(40)-H(40)	119.9
C(40)-C(41)-C(36)	120.1(4)
C(40)-C(41)-H(41)	119.9
C(36)-C(41)-H(41)	119.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 2011ncs0393a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	26(1)	20(1)	21(1)	-5(1)	-2(1)	-4(1)
P(1)	24(1)	21(1)	21(1)	-4(1)	-3(1)	-3(1)
P(2)	35(1)	31(1)	30(1)	-5(1)	-8(1)	-8(1)
F(1)	52(2)	52(2)	41(2)	-19(1)	-1(1)	-14(2)
F(2)	51(2)	34(2)	46(2)	-15(1)	-18(1)	-3(1)
F(3)	42(2)	42(2)	52(2)	-10(1)	-20(2)	5(1)
F(4)	48(2)	64(2)	40(2)	2(2)	-9(1)	-25(2)
F(5)	60(2)	56(2)	36(2)	-4(1)	-7(2)	-24(2)
F(6)	48(2)	44(2)	62(2)	-5(2)	-20(2)	-3(2)
N(1)	25(2)	22(2)	27(2)	-5(1)	-4(2)	-5(2)
N(2)	29(2)	20(2)	27(2)	-6(1)	-4(2)	-5(2)
C(1)	30(2)	40(3)	10(2)	-6(2)	0(2)	-6(2)
C(2)	47(3)	32(3)	28(2)	-11(2)	-5(2)	-3(2)
C(3)	56(3)	24(2)	31(2)	-8(2)	-10(2)	-9(2)
C(4)	36(2)	34(3)	26(2)	-4(2)	-9(2)	-18(2)
C(5)	36(3)	32(3)	36(3)	-3(2)	-13(2)	-1(2)
C(6)	42(3)	29(3)	28(2)	-4(2)	-6(2)	-2(2)
C(7)	36(2)	30(2)	18(2)	3(2)	-4(2)	-11(2)
C(8)	32(2)	34(3)	26(2)	-9(2)	-5(2)	-13(2)
C(9)	19(2)	24(2)	20(2)	-3(2)	-1(2)	-3(2)
C(10)	26(2)	26(2)	35(2)	-7(2)	-6(2)	-8(2)
C(11)	27(2)	24(2)	32(2)	-6(2)	-7(2)	-3(2)
C(12)	24(2)	21(2)	27(2)	-5(2)	-6(2)	-2(2)
C(13)	32(2)	21(2)	35(2)	-4(2)	-5(2)	-4(2)
C(14)	32(2)	23(2)	50(3)	-1(2)	-10(2)	-1(2)
C(15)	39(3)	27(3)	55(3)	-16(2)	-8(2)	2(2)
C(16)	33(3)	34(3)	38(3)	-17(2)	-4(2)	0(2)
C(17)	29(2)	29(2)	31(2)	-11(2)	-2(2)	-4(2)
C(18)	27(2)	21(2)	30(2)	-8(2)	-3(2)	1(2)
C(19)	34(2)	28(2)	29(2)	-5(2)	3(2)	-4(2)
C(20)	38(3)	38(3)	37(3)	-15(2)	9(2)	-4(2)
C(21)	29(2)	38(3)	55(3)	-15(2)	-3(2)	4(2)
C(22)	32(2)	26(3)	43(3)	-6(2)	-4(2)	0(2)
C(23)	29(2)	29(3)	30(2)	-2(2)	-7(2)	0(2)
C(24)	28(2)	25(2)	23(2)	-8(2)	-2(2)	-4(2)
C(25)	29(2)	27(2)	28(2)	-5(2)	-3(2)	-3(2)
C(26)	31(2)	38(3)	28(2)	-8(2)	-3(2)	3(2)
C(27)	23(2)	47(3)	31(2)	-2(2)	-3(2)	-6(2)
C(28)	33(2)	38(3)	33(2)	3(2)	-10(2)	-13(2)
C(29)	32(2)	27(2)	26(2)	-1(2)	-3(2)	-7(2)
C(30)	27(2)	23(2)	23(2)	-2(2)	-5(2)	-3(2)
C(31)	29(2)	23(2)	27(2)	-4(2)	-4(2)	-2(2)
C(32)	36(2)	29(2)	29(2)	-3(2)	-8(2)	-7(2)
C(33)	44(3)	30(3)	26(2)	-7(2)	-11(2)	-7(2)
C(34)	37(3)	38(3)	28(2)	-14(2)	-2(2)	-4(2)
C(35)	31(2)	32(3)	25(2)	-9(2)	0(2)	-5(2)

C(36)	20(2)	24(2)	33(2)	-6(2)	-6(2)	-2(2)
C(37)	30(2)	27(2)	30(2)	-5(2)	-4(2)	-4(2)
C(38)	31(2)	26(2)	42(3)	-9(2)	-6(2)	-5(2)
C(39)	30(2)	27(3)	50(3)	0(2)	-11(2)	-4(2)
C(40)	38(3)	32(3)	42(3)	6(2)	-15(2)	-9(2)
C(41)	33(2)	27(2)	28(2)	1(2)	-3(2)	-5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2011ncs0393a.

	x	y	z	U(eq)
H(1)	5057	7802	580	33
H(2A)	4825	6545	-353	44
H(2B)	3506	7413	-486	44
H(3A)	2644	5899	275	44
H(3B)	3789	5486	762	44
H(4)	2277	6316	1901	36
H(5A)	440	9015	585	41
H(5B)	1595	8075	57	41
H(6A)	2376	9785	-344	41
H(6B)	1778	10266	583	41
H(7)	3858	9658	715	34
H(8)	1034	8188	1875	36
H(10)	5711	10874	2522	34
H(11)	7417	9091	2141	33
H(12)	2512	10432	2279	29
H(13A)	3613	11602	1121	36
H(13B)	4120	12223	1755	36
H(14A)	2311	13543	1399	43
H(14B)	1436	12529	1687	43
H(15A)	858	13804	2778	49
H(15B)	2354	13643	2811	49
H(16A)	1296	12436	3959	42
H(16B)	812	11802	3320	42
H(17A)	2634	10518	3693	36
H(17B)	3489	11546	3383	36
H(18)	6076	6758	1491	32
H(19A)	8345	7849	981	39
H(19B)	7438	7744	374	39
H(20A)	8142	5646	429	49
H(20B)	9404	6261	117	49
H(21A)	9745	5914	1507	51
H(21B)	9713	4671	1183	51
H(22A)	7516	4769	1971	43
H(22B)	8401	4839	2602	43
H(23A)	7708	6918	2587	36

H(23B)	6445	6304	2864	36
H(25)	206	8812	3237	35
H(26)	-1985	8659	3787	41
H(27)	-2548	6805	4346	42
H(28)	-918	5119	4383	41
H(29)	1297	5265	3866	35
H(31)	4835	7902	3510	33
H(32)	5219	8775	4598	37
H(33)	3475	9454	5740	39
H(34)	1369	9230	5794	42
H(35)	990	8329	4703	36
H(37)	4245	5479	2038	35
H(38)	5600	3621	2208	40
H(39)	5832	2823	3562	43
H(40)	4698	3865	4757	44
H(41)	3314	5697	4598	36

Table 6. Torsion angles [°] for 2011ncs0393a.

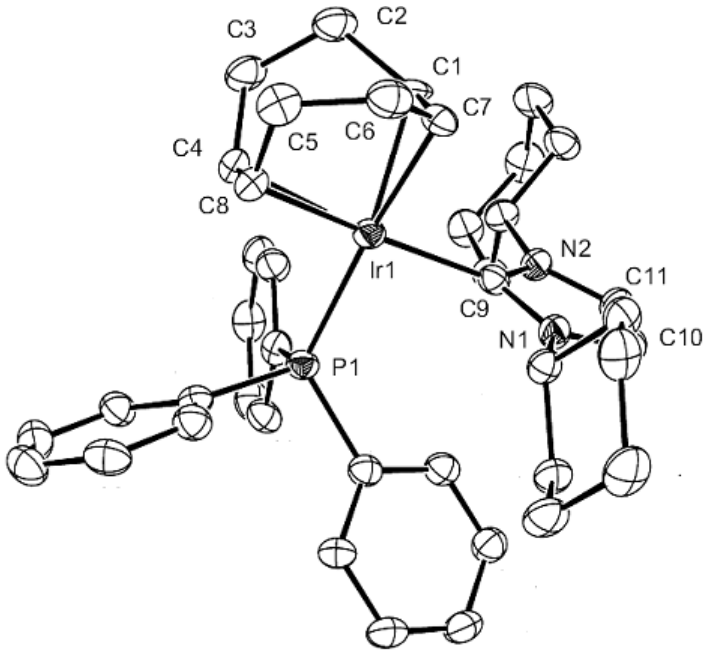
C(9)-Ir(1)-P(1)-C(24)	151.34(19)
C(1)-Ir(1)-P(1)-C(24)	-109.1(3)
C(7)-Ir(1)-P(1)-C(24)	63.5(6)
C(4)-Ir(1)-P(1)-C(24)	-45.6(2)
C(8)-Ir(1)-P(1)-C(24)	-10.3(2)
C(9)-Ir(1)-P(1)-C(36)	-89.53(19)
C(1)-Ir(1)-P(1)-C(36)	10.0(3)
C(7)-Ir(1)-P(1)-C(36)	-177.4(6)
C(4)-Ir(1)-P(1)-C(36)	73.53(19)
C(8)-Ir(1)-P(1)-C(36)	108.84(19)
C(9)-Ir(1)-P(1)-C(30)	27.2(2)
C(1)-Ir(1)-P(1)-C(30)	126.7(3)
C(7)-Ir(1)-P(1)-C(30)	-60.7(6)
C(4)-Ir(1)-P(1)-C(30)	-169.7(2)
C(8)-Ir(1)-P(1)-C(30)	-134.4(2)
C(9)-Ir(1)-C(1)-C(7)	-83.4(3)
C(4)-Ir(1)-C(1)-C(7)	112.1(3)
C(8)-Ir(1)-C(1)-C(7)	76.2(3)
P(1)-Ir(1)-C(1)-C(7)	177.2(2)
C(9)-Ir(1)-C(1)-C(2)	155.2(3)
C(7)-Ir(1)-C(1)-C(2)	-121.3(5)
C(4)-Ir(1)-C(1)-C(2)	-9.3(3)
C(8)-Ir(1)-C(1)-C(2)	-45.2(3)
P(1)-Ir(1)-C(1)-C(2)	55.9(5)
C(7)-C(1)-C(2)-C(3)	-91.5(5)
Ir(1)-C(1)-C(2)-C(3)	-7.1(5)
C(1)-C(2)-C(3)-C(4)	28.7(6)
C(2)-C(3)-C(4)-C(8)	45.4(6)
C(2)-C(3)-C(4)-Ir(1)	-35.2(5)

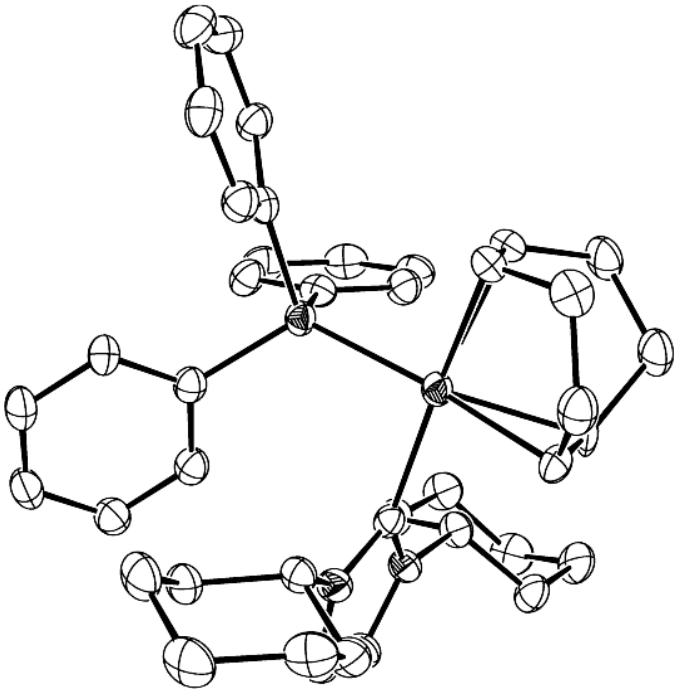
C(9)-Ir(1)-C(4)-C(8)	-163.7(5)
C(1)-Ir(1)-C(4)-C(8)	-97.6(3)
C(7)-Ir(1)-C(4)-C(8)	-63.9(3)
P(1)-Ir(1)-C(4)-C(8)	103.9(3)
C(9)-Ir(1)-C(4)-C(3)	-42.4(7)
C(1)-Ir(1)-C(4)-C(3)	23.7(3)
C(7)-Ir(1)-C(4)-C(3)	57.4(4)
C(8)-Ir(1)-C(4)-C(3)	121.3(5)
P(1)-Ir(1)-C(4)-C(3)	-134.9(3)
C(8)-C(5)-C(6)-C(7)	37.1(5)
C(2)-C(1)-C(7)-C(6)	5.5(7)
Ir(1)-C(1)-C(7)-C(6)	-101.0(4)
C(2)-C(1)-C(7)-Ir(1)	106.5(4)
C(5)-C(6)-C(7)-C(1)	40.6(6)
C(5)-C(6)-C(7)-Ir(1)	-39.6(4)
C(9)-Ir(1)-C(7)-C(1)	96.7(3)
C(4)-Ir(1)-C(7)-C(1)	-66.6(3)
C(8)-Ir(1)-C(7)-C(1)	-99.2(3)
P(1)-Ir(1)-C(7)-C(1)	-175.0(4)
C(9)-Ir(1)-C(7)-C(6)	-140.8(3)
C(1)-Ir(1)-C(7)-C(6)	122.5(4)
C(4)-Ir(1)-C(7)-C(6)	55.9(3)
C(8)-Ir(1)-C(7)-C(6)	23.2(3)
P(1)-Ir(1)-C(7)-C(6)	-52.6(7)
C(3)-C(4)-C(8)-C(5)	5.3(7)
Ir(1)-C(4)-C(8)-C(5)	106.0(4)
C(3)-C(4)-C(8)-Ir(1)	-100.7(4)
C(6)-C(5)-C(8)-C(4)	-98.4(5)
C(6)-C(5)-C(8)-Ir(1)	-16.1(5)
C(9)-Ir(1)-C(8)-C(4)	166.4(4)
C(1)-Ir(1)-C(8)-C(4)	78.3(3)
C(7)-Ir(1)-C(8)-C(4)	114.4(3)
P(1)-Ir(1)-C(8)-C(4)	-78.2(3)
C(9)-Ir(1)-C(8)-C(5)	48.2(6)
C(1)-Ir(1)-C(8)-C(5)	-39.9(3)
C(7)-Ir(1)-C(8)-C(5)	-3.8(3)
C(4)-Ir(1)-C(8)-C(5)	-118.2(4)
P(1)-Ir(1)-C(8)-C(5)	163.6(3)
C(11)-N(2)-C(9)-N(1)	1.9(5)
C(18)-N(2)-C(9)-N(1)	179.7(4)
C(11)-N(2)-C(9)-Ir(1)	178.8(3)
C(18)-N(2)-C(9)-Ir(1)	-3.4(6)
C(10)-N(1)-C(9)-N(2)	-1.7(5)
C(12)-N(1)-C(9)-N(2)	175.6(4)
C(10)-N(1)-C(9)-Ir(1)	-178.8(3)
C(12)-N(1)-C(9)-Ir(1)	-1.5(6)
C(1)-Ir(1)-C(9)-N(2)	-62.0(4)
C(7)-Ir(1)-C(9)-N(2)	-98.3(4)
C(4)-Ir(1)-C(9)-N(2)	2.5(8)
C(8)-Ir(1)-C(9)-N(2)	-149.1(4)
P(1)-Ir(1)-C(9)-N(2)	94.6(4)
C(1)-Ir(1)-C(9)-N(1)	114.3(4)

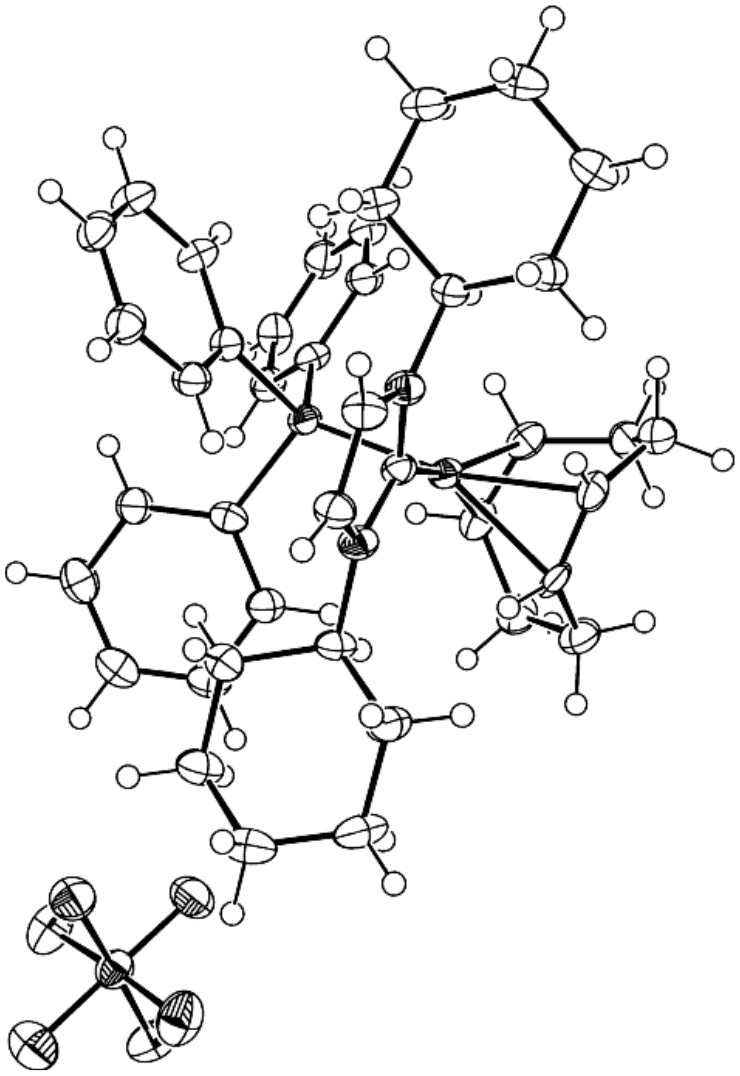
C(7)-Ir(1)-C(9)-N(1)	78.0(4)
C(4)-Ir(1)-C(9)-N(1)	178.8(4)
C(8)-Ir(1)-C(9)-N(1)	27.2(7)
P(1)-Ir(1)-C(9)-N(1)	-89.1(3)
C(9)-N(1)-C(10)-C(11)	0.9(5)
C(12)-N(1)-C(10)-C(11)	-176.5(4)
N(1)-C(10)-C(11)-N(2)	0.3(5)
C(9)-N(2)-C(11)-C(10)	-1.5(5)
C(18)-N(2)-C(11)-C(10)	-179.3(4)
C(9)-N(1)-C(12)-C(17)	124.0(4)
C(10)-N(1)-C(12)-C(17)	-59.1(5)
C(9)-N(1)-C(12)-C(13)	-113.6(4)
C(10)-N(1)-C(12)-C(13)	63.4(5)
N(1)-C(12)-C(13)-C(14)	-178.6(4)
C(17)-C(12)-C(13)-C(14)	-55.9(5)
C(12)-C(13)-C(14)-C(15)	54.9(5)
C(13)-C(14)-C(15)-C(16)	-54.4(5)
C(14)-C(15)-C(16)-C(17)	55.7(5)
C(15)-C(16)-C(17)-C(12)	-56.6(5)
N(1)-C(12)-C(17)-C(16)	178.0(4)
C(13)-C(12)-C(17)-C(16)	56.5(5)
C(9)-N(2)-C(18)-C(19)	122.8(4)
C(11)-N(2)-C(18)-C(19)	-59.7(5)
C(9)-N(2)-C(18)-C(23)	-114.8(5)
C(11)-N(2)-C(18)-C(23)	62.7(5)
N(2)-C(18)-C(19)-C(20)	175.3(4)
C(23)-C(18)-C(19)-C(20)	53.4(5)
C(18)-C(19)-C(20)-C(21)	-56.2(6)
C(19)-C(20)-C(21)-C(22)	57.9(6)
C(20)-C(21)-C(22)-C(23)	-58.3(6)
C(21)-C(22)-C(23)-C(18)	56.2(5)
N(2)-C(18)-C(23)-C(22)	-175.2(4)
C(19)-C(18)-C(23)-C(22)	-53.5(5)
C(36)-P(1)-C(24)-C(25)	179.2(3)
C(30)-P(1)-C(24)-C(25)	73.9(4)
Ir(1)-P(1)-C(24)-C(25)	-59.0(4)
C(36)-P(1)-C(24)-C(29)	0.3(4)
C(30)-P(1)-C(24)-C(29)	-104.9(4)
Ir(1)-P(1)-C(24)-C(29)	122.1(3)
C(29)-C(24)-C(25)-C(26)	2.1(6)
P(1)-C(24)-C(25)-C(26)	-176.8(3)
C(24)-C(25)-C(26)-C(27)	-1.8(7)
C(25)-C(26)-C(27)-C(28)	0.6(7)
C(26)-C(27)-C(28)-C(29)	0.3(7)
C(25)-C(24)-C(29)-C(28)	-1.2(6)
P(1)-C(24)-C(29)-C(28)	177.6(3)
C(27)-C(28)-C(29)-C(24)	0.0(7)
C(24)-P(1)-C(30)-C(35)	-7.1(4)
C(36)-P(1)-C(30)-C(35)	-115.7(4)
Ir(1)-P(1)-C(30)-C(35)	123.0(4)
C(24)-P(1)-C(30)-C(31)	171.2(3)
C(36)-P(1)-C(30)-C(31)	62.7(4)

Ir(1)-P(1)-C(30)-C(31)	-58.7(4)
C(35)-C(30)-C(31)-C(32)	0.6(7)
P(1)-C(30)-C(31)-C(32)	-177.8(3)
C(30)-C(31)-C(32)-C(33)	-0.7(7)
C(31)-C(32)-C(33)-C(34)	0.4(7)
C(32)-C(33)-C(34)-C(35)	0.0(7)
C(31)-C(30)-C(35)-C(34)	-0.2(7)
P(1)-C(30)-C(35)-C(34)	178.1(4)
C(33)-C(34)-C(35)-C(30)	-0.1(7)
C(24)-P(1)-C(36)-C(37)	107.3(4)
C(30)-P(1)-C(36)-C(37)	-146.2(4)
Ir(1)-P(1)-C(36)-C(37)	-17.9(4)
C(24)-P(1)-C(36)-C(41)	-75.0(4)
C(30)-P(1)-C(36)-C(41)	31.5(4)
Ir(1)-P(1)-C(36)-C(41)	159.8(3)
C(41)-C(36)-C(37)-C(38)	-0.7(7)
P(1)-C(36)-C(37)-C(38)	177.1(3)
C(36)-C(37)-C(38)-C(39)	-0.2(7)
C(37)-C(38)-C(39)-C(40)	0.4(7)
C(38)-C(39)-C(40)-C(41)	0.3(7)
C(39)-C(40)-C(41)-C(36)	-1.2(7)
C(37)-C(36)-C(41)-C(40)	1.4(7)
P(1)-C(36)-C(41)-C(40)	-176.3(3)

Symmetry transformations used to generate equivalent atoms:







View with PF_6 anion. All structures omit hydrogen atoms.

8.2 Crystal data for 135

Table 1. Crystal data and structure refinement for 2011ncs0396.

Identification code	2011ncs0396	
Empirical formula	C45 H60.50 F6 Ir N2 O0.75 P2	
Formula weight	1009.59	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.6850(11) Å	α= 90°.
	b = 12.9158(5) Å	β= 115.673(8)°.
	c = 24.6999(17) Å	γ = 90°.
Volume	8535.2(7) $Å^3$	
Z	8	
Density (calculated)	1.571 Mg/m^3	
Absorption coefficient	3.266 mm^{-1}	
F(000)	4092	
Crystal size	0.09 x 0.02 x 0.02 mm^3	
Theta range for data collection	3.05 to 27.48°.	
Index ranges	-38<=h<=38, -16<=k<=16, -29<=l<=32	
Reflections collected	22292	
Independent reflections	9648 [R(int) = 0.0380]	
Completeness to theta = 27.00°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.693	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9648 / 110 / 558	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0794	
R indices (all data)	R1 = 0.0447, wR2 = 0.0848	
Largest diff. peak and hole	2.041 and -1.693 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2011ncs0396. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	3081(1)	2331(1)	1674(1)	16(1)
P(1)	3478(1)	3089(1)	2612(1)	18(1)
P(2)	-1093(1)	2741(3)	491(2)	34(1)
F(1)	-879(3)	3830(4)	808(3)	77(2)
F(2)	-1026(3)	3055(6)	-94(3)	94(2)

F(3)	-1322(2)	1665(3)	182(2)	61(1)
F(4)	-1197(2)	2428(4)	1044(2)	74(2)
F(5)	-1639(2)	3218(4)	177(2)	73(2)
F(6)	-556(2)	2201(8)	811(4)	97(3)
N(1)	2463(1)	4258(2)	1032(1)	18(1)
N(2)	3201(1)	4329(2)	1080(1)	20(1)
C(1)	2986(2)	844(3)	2038(2)	20(1)
C(2)	2509(2)	345(3)	1604(2)	25(1)
C(3)	2414(2)	467(3)	949(2)	26(1)
C(4)	2587(2)	1504(3)	831(2)	22(1)
C(5)	3054(2)	1668(3)	843(2)	24(1)
C(6)	3462(2)	880(3)	993(2)	30(1)
C(7)	3552(2)	232(3)	1555(2)	28(1)
C(8)	3444(2)	819(3)	2018(2)	22(1)
C(9)	2905(2)	3742(3)	1245(2)	19(1)
C(10)	2488(2)	5152(3)	730(2)	24(1)
C(11)	2946(2)	5195(3)	760(2)	26(1)
C(12)	2011(2)	3931(3)	1092(2)	20(1)
C(13)	1852(2)	4735(3)	1426(2)	26(1)
C(14)	1382(2)	4397(4)	1484(2)	29(1)
C(15)	957(2)	4142(4)	875(2)	32(1)
C(16)	1124(2)	3338(4)	543(2)	33(1)
C(17)	1585(2)	3707(3)	479(2)	25(1)
C(18)	3713(2)	4058(3)	1186(2)	20(1)
C(19)	4091(2)	4866(3)	1580(2)	24(1)
C(20)	4621(2)	4583(3)	1679(2)	26(1)
C(21)	4650(2)	4423(3)	1084(2)	24(1)
C(22)	4281(2)	3591(3)	713(2)	22(1)
C(23)	3752(2)	3909(3)	593(2)	20(1)
C(24)	3396(2)	2451(3)	3228(2)	21(1)
C(25)	2885(2)	2514(3)	3217(2)	23(1)
C(26)	2440(2)	2420(3)	2698(2)	28(1)
C(27)	1982(2)	2410(3)	2719(2)	36(1)
C(28)	1956(2)	2517(4)	3263(3)	39(1)
C(29)	2389(2)	2634(3)	3782(2)	37(1)
C(30)	2850(2)	2632(3)	3761(2)	29(1)
C(31)	3332(2)	4469(3)	2689(2)	21(1)
C(32)	3708(2)	5005(3)	3245(2)	22(1)
C(33)	3749(2)	4771(3)	3816(2)	26(1)
C(34)	4125(2)	5198(4)	4327(2)	35(1)
C(35)	4456(2)	5885(4)	4280(2)	37(1)
C(36)	4417(2)	6162(4)	3718(2)	33(1)
C(37)	4045(2)	5716(3)	3203(2)	28(1)
C(38)	4169(2)	3115(3)	2875(2)	22(1)
C(39)	4476(3)	2247(6)	3286(3)	27(1)
C(40)	4575(3)	2234(6)	3894(3)	34(2)
C(41)	4872(3)	1452(6)	4270(4)	52(2)
C(42)	5074(3)	687(6)	4038(5)	63(2)
C(43)	4991(3)	718(6)	3451(5)	58(2)
C(44)	4687(3)	1492(6)	3064(4)	39(2)
O(1S)	0	3322(7)	2500	33(2)
C(1S)	-342(5)	2675(9)	2591(6)	45(3)

C(2S)	-636(4)	3352(7)	2812(6)	45(3)
O(2S)	-471(3)	3183(6)	2581(3)	33(2)
C(39A)	4487(8)	2198(12)	3137(7)	27(1)
C(40A)	4626(7)	1941(14)	3735(7)	34(2)
C(41A)	4909(7)	1057(15)	3977(7)	52(2)
C(42A)	5053(6)	430(12)	3622(9)	63(2)
C(43A)	4914(6)	688(11)	3024(9)	58(2)
C(44A)	4631(7)	1572(13)	2782(6)	39(2)
P(3)	-979(4)	2784(9)	432(5)	34(1)
F(7)	-1321(6)	3570(12)	-50(7)	73(2)
F(8)	-1481(6)	2276(13)	394(7)	74(2)
F(9)	-965(6)	1946(9)	-30(5)	61(1)
F(10)	-484(6)	3266(15)	486(7)	94(2)
F(11)	-686(8)	2080(20)	991(10)	97(3)
F(12)	-990(10)	3538(14)	924(10)	77(2)

Table 3. Bond lengths [Å] and angles [°] for 2011ncs0396.

Ir(1)-C(9)	2.059(4)
Ir(1)-C(1)	2.190(3)
Ir(1)-C(5)	2.194(4)
Ir(1)-C(8)	2.214(4)
Ir(1)-C(4)	2.233(4)
Ir(1)-P(1)	2.3109(9)
P(1)-C(24)	1.839(4)
P(1)-C(31)	1.863(4)
P(1)-C(38)	1.865(4)
P(2)-F(4)	1.578(6)
P(2)-F(5)	1.587(5)
P(2)-F(3)	1.589(5)
P(2)-F(2)	1.592(6)
P(2)-F(6)	1.600(6)
P(2)-F(1)	1.602(6)
N(1)-C(9)	1.360(5)
N(1)-C(10)	1.393(5)
N(1)-C(12)	1.471(5)
N(2)-C(9)	1.350(5)
N(2)-C(11)	1.389(5)
N(2)-C(18)	1.469(5)
C(1)-C(8)	1.383(6)
C(1)-C(2)	1.503(5)
C(1)-H(1)	0.9500
C(2)-C(3)	1.525(5)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.507(5)
C(3)-H(3A)	0.9900

C(3)-H(3B)	0.9900
C(4)-C(5)	1.391(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.500(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.540(6)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.519(6)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8)	0.9500
C(10)-C(11)	1.332(6)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(17)	1.523(5)
C(12)-C(13)	1.524(5)
C(12)-H(12)	1.0000
C(13)-C(14)	1.526(6)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.523(6)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.533(6)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.521(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(23)	1.528(5)
C(18)-C(19)	1.533(5)
C(18)-H(18)	1.0000
C(19)-C(20)	1.528(6)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.526(6)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.524(5)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.525(6)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.509(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900

C(25)-C(26)	1.392(6)
C(25)-C(30)	1.399(6)
C(26)-C(27)	1.381(7)
C(26)-H(26)	0.9500
C(27)-C(28)	1.386(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.375(8)
C(28)-H(28)	0.9500
C(29)-C(30)	1.390(7)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(32)	1.510(5)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(37)	1.395(6)
C(32)-C(33)	1.396(6)
C(33)-C(34)	1.388(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.366(7)
C(34)-H(34)	0.9500
C(35)-C(36)	1.389(7)
C(35)-H(35)	0.9500
C(36)-C(37)	1.397(6)
C(36)-H(36)	0.9500
C(37)-H(37)	0.9500
C(38)-C(39A)	1.478(12)
C(38)-C(39)	1.523(7)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(44)	1.393(9)
C(39)-C(40)	1.400(9)
C(40)-C(41)	1.396(9)
C(40)-H(40)	0.9500
C(41)-C(42)	1.400(13)
C(41)-H(41)	0.9500
C(42)-C(43)	1.363(14)
C(42)-H(42)	0.9500
C(43)-C(44)	1.407(11)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
O(1S)-C(1S)	1.405(8)
O(1S)-C(1S)#1	1.405(8)
O(1S)-H(1W)	1.0188
C(1S)-C(2S)	1.497(9)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900
C(1S)-H(1W)	0.6860
C(1S)-H(2W)	0.8607
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800
C(2S)-H(2S3)	0.9800
C(2S)-H(2W)	1.2205

O(2S)-H(1W)	0.9621
O(2S)-H(2W)	0.8886
C(39A)-C(40A)	1.3900
C(39A)-C(44A)	1.3900
C(40A)-C(41A)	1.3900
C(40A)-H(40A)	0.9500
C(41A)-C(42A)	1.3900
C(41A)-H(41A)	0.9500
C(42A)-C(43A)	1.3900
C(42A)-H(42A)	0.9500
C(43A)-C(44A)	1.3900
C(43A)-H(43A)	0.9500
C(44A)-H(44A)	0.9500
P(3)-F(10)	1.547(14)
P(3)-F(7)	1.560(14)
P(3)-F(11)	1.567(18)
P(3)-F(12)	1.569(17)
P(3)-F(9)	1.588(13)
P(3)-F(8)	1.594(14)

C(9)-Ir(1)-C(1)	159.82(16)
C(9)-Ir(1)-C(5)	87.99(14)
C(1)-Ir(1)-C(5)	94.74(14)
C(9)-Ir(1)-C(8)	161.94(16)
C(1)-Ir(1)-C(8)	36.59(15)
C(5)-Ir(1)-C(8)	80.10(15)
C(9)-Ir(1)-C(4)	91.41(14)
C(1)-Ir(1)-C(4)	79.29(14)
C(5)-Ir(1)-C(4)	36.61(16)
C(8)-Ir(1)-C(4)	87.09(14)
C(9)-Ir(1)-P(1)	92.72(10)
C(1)-Ir(1)-P(1)	93.48(10)
C(5)-Ir(1)-P(1)	153.97(12)
C(8)-Ir(1)-P(1)	92.15(10)
C(4)-Ir(1)-P(1)	168.81(11)
C(24)-P(1)-C(31)	102.89(18)
C(24)-P(1)-C(38)	103.92(18)
C(31)-P(1)-C(38)	102.47(18)
C(24)-P(1)-Ir(1)	116.55(13)
C(31)-P(1)-Ir(1)	117.88(12)
C(38)-P(1)-Ir(1)	111.32(13)
F(4)-P(2)-F(5)	88.9(3)
F(4)-P(2)-F(3)	89.3(3)
F(5)-P(2)-F(3)	88.4(3)
F(4)-P(2)-F(2)	176.3(4)
F(5)-P(2)-F(2)	87.7(4)
F(3)-P(2)-F(2)	89.0(3)
F(4)-P(2)-F(6)	89.3(4)
F(5)-P(2)-F(6)	176.9(5)
F(3)-P(2)-F(6)	89.0(4)
F(2)-P(2)-F(6)	94.0(5)
F(4)-P(2)-F(1)	89.2(4)

F(5)-P(2)-F(1)	90.1(4)
F(3)-P(2)-F(1)	177.9(4)
F(2)-P(2)-F(1)	92.4(4)
F(6)-P(2)-F(1)	92.4(5)
C(9)-N(1)-C(10)	110.2(3)
C(9)-N(1)-C(12)	126.1(3)
C(10)-N(1)-C(12)	123.6(3)
C(9)-N(2)-C(11)	110.9(3)
C(9)-N(2)-C(18)	124.9(3)
C(11)-N(2)-C(18)	124.1(3)
C(8)-C(1)-C(2)	127.0(4)
C(8)-C(1)-Ir(1)	72.6(2)
C(2)-C(1)-Ir(1)	109.4(2)
C(8)-C(1)-H(1)	116.5
C(2)-C(1)-H(1)	116.5
Ir(1)-C(1)-H(1)	87.8
C(1)-C(2)-C(3)	113.4(3)
C(1)-C(2)-H(2A)	108.9
C(3)-C(2)-H(2A)	108.9
C(1)-C(2)-H(2B)	108.9
C(3)-C(2)-H(2B)	108.9
H(2A)-C(2)-H(2B)	107.7
C(4)-C(3)-C(2)	112.0(3)
C(4)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3B)	109.2
C(2)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
C(5)-C(4)-C(3)	123.4(4)
C(5)-C(4)-Ir(1)	70.2(2)
C(3)-C(4)-Ir(1)	112.7(2)
C(5)-C(4)-H(4)	118.3
C(3)-C(4)-H(4)	118.3
Ir(1)-C(4)-H(4)	87.2
C(4)-C(5)-C(6)	126.4(4)
C(4)-C(5)-Ir(1)	73.2(2)
C(6)-C(5)-Ir(1)	109.6(3)
C(4)-C(5)-H(5)	116.8
C(6)-C(5)-H(5)	116.8
Ir(1)-C(5)-H(5)	87.0
C(5)-C(6)-C(7)	113.5(4)
C(5)-C(6)-H(6A)	108.9
C(7)-C(6)-H(6A)	108.9
C(5)-C(6)-H(6B)	108.9
C(7)-C(6)-H(6B)	108.9
H(6A)-C(6)-H(6B)	107.7
C(8)-C(7)-C(6)	113.3(3)
C(8)-C(7)-H(7A)	108.9
C(6)-C(7)-H(7A)	108.9
C(8)-C(7)-H(7B)	108.9
C(6)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.7

C(1)-C(8)-C(7)	124.9(4)
C(1)-C(8)-Ir(1)	70.8(2)
C(7)-C(8)-Ir(1)	112.3(2)
C(1)-C(8)-H(8)	117.6
C(7)-C(8)-H(8)	117.6
Ir(1)-C(8)-H(8)	86.9
N(2)-C(9)-N(1)	104.8(3)
N(2)-C(9)-Ir(1)	126.8(3)
N(1)-C(9)-Ir(1)	128.3(3)
C(11)-C(10)-N(1)	107.2(4)
C(11)-C(10)-H(10)	126.4
N(1)-C(10)-H(10)	126.4
C(10)-C(11)-N(2)	106.9(4)
C(10)-C(11)-H(11)	126.6
N(2)-C(11)-H(11)	126.6
N(1)-C(12)-C(17)	110.7(3)
N(1)-C(12)-C(13)	111.6(3)
C(17)-C(12)-C(13)	110.5(3)
N(1)-C(12)-H(12)	108.0
C(17)-C(12)-H(12)	108.0
C(13)-C(12)-H(12)	108.0
C(12)-C(13)-C(14)	111.5(3)
C(12)-C(13)-H(13A)	109.3
C(14)-C(13)-H(13A)	109.3
C(12)-C(13)-H(13B)	109.3
C(14)-C(13)-H(13B)	109.3
H(13A)-C(13)-H(13B)	108.0
C(15)-C(14)-C(13)	111.8(4)
C(15)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14B)	109.3
C(13)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	107.9
C(14)-C(15)-C(16)	110.6(4)
C(14)-C(15)-H(15A)	109.5
C(16)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
C(16)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	108.1
C(17)-C(16)-C(15)	111.0(4)
C(17)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16B)	109.4
C(15)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(16)-C(17)-C(12)	110.6(3)
C(16)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	108.1
N(2)-C(18)-C(23)	111.1(3)

N(2)-C(18)-C(19)	111.4(3)
C(23)-C(18)-C(19)	111.0(3)
N(2)-C(18)-H(18)	107.7
C(23)-C(18)-H(18)	107.7
C(19)-C(18)-H(18)	107.7
C(20)-C(19)-C(18)	110.9(3)
C(20)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19A)	109.5
C(20)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	108.0
C(21)-C(20)-C(19)	111.3(3)
C(21)-C(20)-H(20A)	109.4
C(19)-C(20)-H(20A)	109.4
C(21)-C(20)-H(20B)	109.4
C(19)-C(20)-H(20B)	109.4
H(20A)-C(20)-H(20B)	108.0
C(22)-C(21)-C(20)	110.4(3)
C(22)-C(21)-H(21A)	109.6
C(20)-C(21)-H(21A)	109.6
C(22)-C(21)-H(21B)	109.6
C(20)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1
C(21)-C(22)-C(23)	109.8(3)
C(21)-C(22)-H(22A)	109.7
C(23)-C(22)-H(22A)	109.7
C(21)-C(22)-H(22B)	109.7
C(23)-C(22)-H(22B)	109.7
H(22A)-C(22)-H(22B)	108.2
C(22)-C(23)-C(18)	110.2(3)
C(22)-C(23)-H(23A)	109.6
C(18)-C(23)-H(23A)	109.6
C(22)-C(23)-H(23B)	109.6
C(18)-C(23)-H(23B)	109.6
H(23A)-C(23)-H(23B)	108.1
C(25)-C(24)-P(1)	117.1(3)
C(25)-C(24)-H(24A)	108.0
P(1)-C(24)-H(24A)	108.0
C(25)-C(24)-H(24B)	108.0
P(1)-C(24)-H(24B)	108.0
H(24A)-C(24)-H(24B)	107.3
C(26)-C(25)-C(30)	117.4(4)
C(26)-C(25)-C(24)	123.9(4)
C(30)-C(25)-C(24)	118.7(4)
C(27)-C(26)-C(25)	121.5(4)
C(27)-C(26)-H(26)	119.3
C(25)-C(26)-H(26)	119.3
C(26)-C(27)-C(28)	120.3(5)
C(26)-C(27)-H(27)	119.9
C(28)-C(27)-H(27)	119.9
C(29)-C(28)-C(27)	119.4(5)
C(29)-C(28)-H(28)	120.3

C(27)-C(28)-H(28)	120.3
C(28)-C(29)-C(30)	120.3(5)
C(28)-C(29)-H(29)	119.9
C(30)-C(29)-H(29)	119.9
C(29)-C(30)-C(25)	121.1(5)
C(29)-C(30)-H(30)	119.4
C(25)-C(30)-H(30)	119.4
C(32)-C(31)-P(1)	114.8(3)
C(32)-C(31)-H(31A)	108.6
P(1)-C(31)-H(31A)	108.6
C(32)-C(31)-H(31B)	108.6
P(1)-C(31)-H(31B)	108.6
H(31A)-C(31)-H(31B)	107.5
C(37)-C(32)-C(33)	117.8(4)
C(37)-C(32)-C(31)	120.4(4)
C(33)-C(32)-C(31)	121.7(4)
C(34)-C(33)-C(32)	121.2(4)
C(34)-C(33)-H(33)	119.4
C(32)-C(33)-H(33)	119.4
C(35)-C(34)-C(33)	120.4(4)
C(35)-C(34)-H(34)	119.8
C(33)-C(34)-H(34)	119.8
C(34)-C(35)-C(36)	120.1(4)
C(34)-C(35)-H(35)	120.0
C(36)-C(35)-H(35)	120.0
C(35)-C(36)-C(37)	119.7(4)
C(35)-C(36)-H(36)	120.2
C(37)-C(36)-H(36)	120.2
C(32)-C(37)-C(36)	120.9(4)
C(32)-C(37)-H(37)	119.5
C(36)-C(37)-H(37)	119.5
C(39A)-C(38)-C(39)	14.8(8)
C(39A)-C(38)-P(1)	122.3(9)
C(39)-C(38)-P(1)	117.9(4)
C(39A)-C(38)-H(38A)	93.3
C(39)-C(38)-H(38A)	107.8
P(1)-C(38)-H(38A)	107.8
C(39A)-C(38)-H(38B)	116.1
C(39)-C(38)-H(38B)	107.8
P(1)-C(38)-H(38B)	107.8
H(38A)-C(38)-H(38B)	107.2
C(44)-C(39)-C(40)	119.5(6)
C(44)-C(39)-C(38)	119.6(6)
C(40)-C(39)-C(38)	120.7(6)
C(41)-C(40)-C(39)	120.0(7)
C(41)-C(40)-H(40)	120.0
C(39)-C(40)-H(40)	120.0
C(40)-C(41)-C(42)	119.9(8)
C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.1
C(43)-C(42)-C(41)	120.1(7)
C(43)-C(42)-H(42)	120.0

C(41)-C(42)-H(42)	120.0
C(42)-C(43)-C(44)	120.7(8)
C(42)-C(43)-H(43)	119.7
C(44)-C(43)-H(43)	119.7
C(39)-C(44)-C(43)	119.8(8)
C(39)-C(44)-H(44)	120.1
C(43)-C(44)-H(44)	120.1
C(1S)-O(1S)-C(1S)#1	107.0(12)
C(1S)-O(1S)-H(1W)	27.4
C(1S)#1-O(1S)-H(1W)	102.6
O(1S)-C(1S)-C(2S)	106.7(8)
O(1S)-C(1S)-H(1S1)	110.4
C(2S)-C(1S)-H(1S1)	110.4
O(1S)-C(1S)-H(1S2)	110.4
C(2S)-C(1S)-H(1S2)	110.4
H(1S1)-C(1S)-H(1S2)	108.6
O(1S)-C(1S)-H(1W)	43.1
C(2S)-C(1S)-H(1W)	113.6
H(1S1)-C(1S)-H(1W)	133.8
H(1S2)-C(1S)-H(1W)	68.3
O(1S)-C(1S)-H(2W)	81.2
C(2S)-C(1S)-H(2W)	54.6
H(1S1)-C(1S)-H(2W)	75.7
H(1S2)-C(1S)-H(2W)	164.2
H(1W)-C(1S)-H(2W)	120.3
C(1S)-C(2S)-H(2W)	35.1
H(2S1)-C(2S)-H(2W)	74.8
H(2S2)-C(2S)-H(2W)	117.7
H(2S3)-C(2S)-H(2W)	128.0
H(1W)-O(2S)-H(2W)	93.1
C(40A)-C(39A)-C(44A)	120.0
C(40A)-C(39A)-C(38)	119.8(11)
C(44A)-C(39A)-C(38)	120.1(11)
C(39A)-C(40A)-C(41A)	120.0
C(39A)-C(40A)-H(40A)	120.0
C(41A)-C(40A)-H(40A)	120.0
C(40A)-C(41A)-C(42A)	120.0
C(40A)-C(41A)-H(41A)	120.0
C(42A)-C(41A)-H(41A)	120.0
C(43A)-C(42A)-C(41A)	120.0
C(43A)-C(42A)-H(42A)	120.0
C(41A)-C(42A)-H(42A)	120.0
C(44A)-C(43A)-C(42A)	120.0
C(44A)-C(43A)-H(43A)	120.0
C(42A)-C(43A)-H(43A)	120.0
C(43A)-C(44A)-C(39A)	120.0
C(43A)-C(44A)-H(44A)	120.0
C(39A)-C(44A)-H(44A)	120.0
F(10)-P(3)-F(7)	94.8(12)
F(10)-P(3)-F(11)	90.9(13)
F(7)-P(3)-F(11)	169.0(13)
F(10)-P(3)-F(12)	91.2(12)

F(7)-P(3)-F(12)	87.9(13)
F(11)-P(3)-F(12)	82.6(15)
F(10)-P(3)-F(9)	91.0(10)
F(7)-P(3)-F(9)	96.0(10)
F(11)-P(3)-F(9)	93.3(12)
F(12)-P(3)-F(9)	175.4(12)
F(10)-P(3)-F(8)	178.5(12)
F(7)-P(3)-F(8)	86.6(11)
F(11)-P(3)-F(8)	87.7(12)
F(12)-P(3)-F(8)	88.2(11)
F(9)-P(3)-F(8)	89.5(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 2011ncs0396. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	20(1)	13(1)	13(1)	0(1)	4(1)	-1(1)
P(1)	19(1)	16(1)	14(1)	0(1)	3(1)	0(1)
P(2)	39(2)	25(1)	37(1)	4(1)	16(1)	4(1)
F(1)	88(5)	32(3)	92(4)	-13(3)	21(3)	-17(3)
F(2)	111(5)	114(5)	73(4)	-1(3)	55(4)	-56(4)
F(3)	79(4)	33(2)	56(3)	-1(2)	16(2)	0(2)
F(4)	87(4)	80(4)	58(3)	8(2)	36(3)	-5(3)
F(5)	56(3)	71(3)	66(3)	-3(3)	2(2)	31(3)
F(6)	37(4)	118(5)	108(6)	-41(4)	4(3)	33(4)
N(1)	21(2)	13(2)	20(2)	1(1)	9(1)	0(1)
N(2)	23(2)	15(2)	22(2)	2(1)	9(1)	1(1)
C(1)	30(2)	11(2)	17(2)	4(1)	8(2)	-2(2)
C(2)	27(2)	21(2)	24(2)	-1(2)	9(2)	-8(2)
C(3)	31(2)	18(2)	20(2)	-2(1)	2(2)	-7(2)
C(4)	31(2)	16(2)	14(2)	-4(1)	4(2)	-3(2)
C(5)	41(3)	13(2)	19(2)	-1(1)	14(2)	-2(2)
C(6)	43(3)	27(2)	29(2)	-1(2)	21(2)	0(2)
C(7)	29(2)	21(2)	34(2)	4(2)	14(2)	6(2)
C(8)	29(2)	9(2)	22(2)	5(1)	4(2)	4(2)
C(9)	26(2)	15(2)	13(2)	-4(1)	8(2)	-3(2)
C(10)	26(2)	17(2)	30(2)	6(2)	12(2)	3(2)
C(11)	30(2)	14(2)	31(2)	7(2)	13(2)	4(2)
C(12)	22(2)	18(2)	20(2)	-1(1)	9(2)	-1(2)
C(13)	27(2)	27(2)	23(2)	-10(2)	10(2)	-4(2)
C(14)	31(2)	30(2)	29(2)	-5(2)	16(2)	0(2)
C(15)	22(2)	33(2)	39(2)	-10(2)	13(2)	-2(2)

C(16)	26(2)	31(2)	36(2)	-16(2)	9(2)	-5(2)
C(17)	24(2)	24(2)	24(2)	-6(2)	8(2)	1(2)
C(18)	22(2)	19(2)	15(2)	0(1)	4(2)	2(2)
C(19)	27(2)	22(2)	22(2)	-4(2)	10(2)	-3(2)
C(20)	22(2)	29(2)	20(2)	0(2)	3(2)	-6(2)
C(21)	20(2)	26(2)	22(2)	5(2)	6(2)	0(2)
C(22)	26(2)	19(2)	20(2)	1(1)	9(2)	2(2)
C(23)	22(2)	22(2)	14(2)	-1(1)	4(2)	-3(2)
C(24)	24(2)	21(2)	14(2)	1(1)	4(2)	1(2)
C(25)	29(2)	13(2)	28(2)	2(1)	13(2)	0(2)
C(26)	27(2)	22(2)	32(2)	4(2)	11(2)	2(2)
C(27)	30(2)	28(2)	48(3)	8(2)	14(2)	-1(2)
C(28)	39(3)	23(2)	67(4)	11(2)	33(3)	2(2)
C(29)	55(3)	20(2)	54(3)	4(2)	41(3)	2(2)
C(30)	43(3)	20(2)	28(2)	3(2)	19(2)	2(2)
C(31)	21(2)	19(2)	19(2)	-2(1)	4(2)	0(2)
C(32)	20(2)	19(2)	22(2)	-5(1)	4(2)	2(2)
C(33)	26(2)	25(2)	24(2)	-4(2)	9(2)	4(2)
C(34)	35(3)	36(3)	24(2)	-11(2)	4(2)	9(2)
C(35)	24(2)	43(3)	33(2)	-22(2)	2(2)	3(2)
C(36)	19(2)	31(2)	49(3)	-20(2)	13(2)	-6(2)
C(37)	26(2)	24(2)	31(2)	-10(2)	11(2)	2(2)
C(38)	19(2)	22(2)	23(2)	1(2)	5(2)	1(2)
C(39)	18(2)	20(2)	36(4)	0(2)	4(3)	-2(2)
C(40)	20(3)	37(4)	34(3)	8(3)	3(2)	-4(3)
C(41)	24(3)	52(4)	58(4)	30(3)	-3(3)	-9(3)
C(42)	31(4)	27(3)	98(5)	24(4)	-3(4)	1(3)
C(43)	28(3)	28(3)	97(5)	-7(4)	7(4)	6(3)
C(44)	18(3)	31(3)	56(4)	-13(3)	5(4)	1(2)
O(1S)	23(5)	40(5)	36(5)	0	12(4)	0
C(1S)	56(8)	23(5)	65(8)	-1(6)	35(7)	-16(6)
C(2S)	40(6)	20(5)	80(9)	12(5)	29(6)	-8(4)
O(2S)	36(5)	31(5)	19(3)	12(3)	0(3)	-1(4)
C(39A)	18(2)	20(2)	36(4)	0(2)	4(3)	-2(2)
C(40A)	20(3)	37(4)	34(3)	8(3)	3(2)	-4(3)
C(41A)	24(3)	52(4)	58(4)	30(3)	-3(3)	-9(3)
C(42A)	31(4)	27(3)	98(5)	24(4)	-3(4)	1(3)
C(43A)	28(3)	28(3)	97(5)	-7(4)	7(4)	6(3)
C(44A)	18(3)	31(3)	56(4)	-13(3)	5(4)	1(2)
P(3)	39(2)	25(1)	37(1)	4(1)	16(1)	4(1)
F(7)	56(3)	71(3)	66(3)	-3(3)	2(2)	31(3)
F(8)	87(4)	80(4)	58(3)	8(2)	36(3)	-5(3)
F(9)	79(4)	33(2)	56(3)	-1(2)	16(2)	0(2)
F(10)	111(5)	114(5)	73(4)	-1(3)	55(4)	-56(4)
F(11)	37(4)	118(5)	108(6)	-41(4)	4(3)	33(4)
F(12)	88(5)	32(3)	92(4)	-13(3)	21(3)	-17(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2011ncs0396.

	x	y	z	U(eq)
H(1)	2972	1217	2362	24
H(2A)	2226	653	1658	29
H(2B)	2520	-403	1698	29
H(3A)	2591	-89	843	32
H(3B)	2051	390	688	32
H(4)	2365	2076	743	27
H(5)	3122	2345	747	29
H(6A)	3776	1240	1059	36
H(6B)	3375	409	646	36
H(7A)	3338	-392	1429	33
H(7B)	3905	-1	1743	33
H(8)	3711	1198	2315	27
H(10)	2226	5639	538	29
H(11)	3074	5718	595	31
H(12)	2092	3275	1331	24
H(13A)	1788	5402	1209	31
H(13B)	2127	4842	1832	31
H(14A)	1459	3779	1746	35
H(14B)	1275	4958	1675	35
H(15A)	848	4781	630	38
H(15B)	669	3869	931	38
H(16A)	1200	2677	768	39
H(16B)	850	3211	140	39
H(17A)	1504	4342	230	30
H(17B)	1691	3168	272	30
H(18)	3799	3383	1406	24
H(19A)	4001	5554	1385	29
H(19B)	4077	4910	1973	29
H(20A)	4853	5143	1908	31
H(20B)	4726	3941	1920	31
H(21A)	4573	5081	856	28
H(21B)	4993	4213	1161	28
H(22A)	4366	2925	933	26
H(22B)	4302	3495	327	26
H(23A)	3513	3369	351	24
H(23B)	3663	4563	361	24
H(24A)	3483	1710	3230	26
H(24B)	3640	2755	3611	26
H(26)	2451	2360	2321	33
H(27)	1684	2330	2359	44
H(28)	1642	2509	3277	47
H(29)	2374	2717	4155	44
H(30)	3147	2712	4123	35
H(31A)	3309	4854	2332	25
H(31B)	3000	4502	2693	25

H(33)	3515	4311	3855	31
H(34)	4153	5011	4713	41
H(35)	4713	6174	4632	44
H(36)	4642	6652	3684	40
H(37)	4022	5899	2819	33
H(38A)	4236	3118	2515	27
H(38B)	4295	3780	3087	27
H(40)	4440	2758	4051	40
H(41)	4937	1439	4681	62
H(42)	5270	145	4291	76
H(43)	5141	213	3301	70
H(44)	4626	1500	2654	47
H(1S1)	-162	2134	2892	54
H(1S2)	-566	2333	2211	54
H(2S1)	-408	3718	3175	68
H(2S2)	-866	2924	2906	68
H(2S3)	-828	3856	2501	68
H(1W)	-314	2878	2350	50
H(2W)	-223	2998	2929	50
H(40A)	4528	2369	3978	40
H(41A)	5004	881	4386	62
H(42A)	5247	-174	3788	76
H(43A)	5013	260	2782	70
H(44A)	4536	1748	2374	47

Table 6. Torsion angles [°] for 2011ncs0396.

C(9)-Ir(1)-P(1)-C(24)	142.33(19)
C(1)-Ir(1)-P(1)-C(24)	-18.46(19)
C(5)-Ir(1)-P(1)-C(24)	-126.7(3)
C(8)-Ir(1)-P(1)-C(24)	-55.07(19)
C(4)-Ir(1)-P(1)-C(24)	30.8(6)
C(9)-Ir(1)-P(1)-C(31)	19.21(19)
C(1)-Ir(1)-P(1)-C(31)	-141.58(19)
C(5)-Ir(1)-P(1)-C(31)	110.2(3)
C(8)-Ir(1)-P(1)-C(31)	-178.19(19)
C(4)-Ir(1)-P(1)-C(31)	-92.3(6)
C(9)-Ir(1)-P(1)-C(38)	-98.74(18)
C(1)-Ir(1)-P(1)-C(38)	100.47(18)
C(5)-Ir(1)-P(1)-C(38)	-7.8(3)
C(8)-Ir(1)-P(1)-C(38)	63.86(18)
C(4)-Ir(1)-P(1)-C(38)	149.8(6)
C(9)-Ir(1)-C(1)-C(8)	163.4(4)
C(5)-Ir(1)-C(1)-C(8)	66.3(2)
C(4)-Ir(1)-C(1)-C(8)	99.7(2)
P(1)-Ir(1)-C(1)-C(8)	-88.9(2)
C(9)-Ir(1)-C(1)-C(2)	39.5(6)

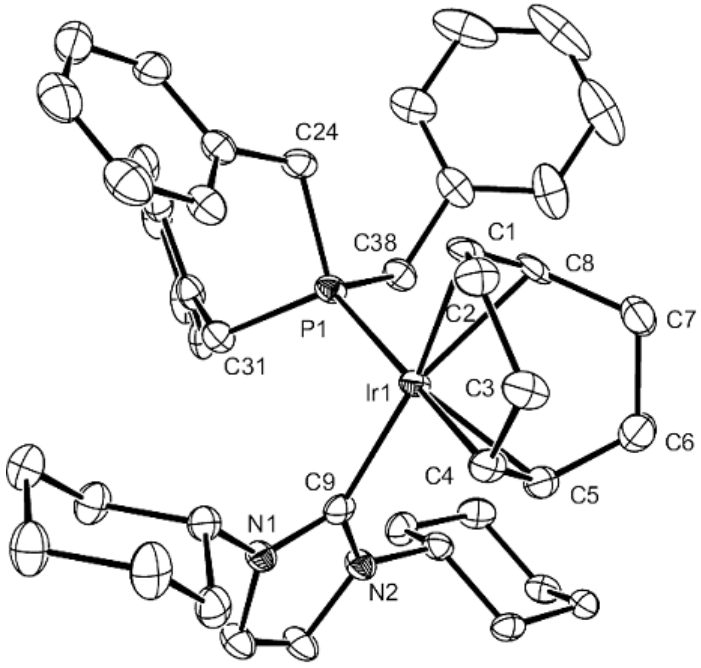
C(5)-Ir(1)-C(1)-C(2)	-57.5(3)
C(8)-Ir(1)-C(1)-C(2)	-123.9(4)
C(4)-Ir(1)-C(1)-C(2)	-24.2(3)
P(1)-Ir(1)-C(1)-C(2)	147.2(3)
C(8)-C(1)-C(2)-C(3)	-42.3(5)
Ir(1)-C(1)-C(2)-C(3)	40.2(4)
C(1)-C(2)-C(3)-C(4)	-36.1(5)
C(2)-C(3)-C(4)-C(5)	94.5(5)
C(2)-C(3)-C(4)-Ir(1)	14.0(5)
C(9)-Ir(1)-C(4)-C(5)	84.7(2)
C(1)-Ir(1)-C(4)-C(5)	-113.3(3)
C(8)-Ir(1)-C(4)-C(5)	-77.3(2)
P(1)-Ir(1)-C(4)-C(5)	-163.7(4)
C(9)-Ir(1)-C(4)-C(3)	-156.3(3)
C(1)-Ir(1)-C(4)-C(3)	5.7(3)
C(5)-Ir(1)-C(4)-C(3)	119.0(4)
C(8)-Ir(1)-C(4)-C(3)	41.7(3)
P(1)-Ir(1)-C(4)-C(3)	-44.7(7)
C(3)-C(4)-C(5)-C(6)	-2.4(6)
Ir(1)-C(4)-C(5)-C(6)	102.3(4)
C(3)-C(4)-C(5)-Ir(1)	-104.7(3)
C(9)-Ir(1)-C(5)-C(4)	-95.1(2)
C(1)-Ir(1)-C(5)-C(4)	64.9(2)
C(8)-Ir(1)-C(5)-C(4)	98.6(2)
P(1)-Ir(1)-C(5)-C(4)	172.85(19)
C(9)-Ir(1)-C(5)-C(6)	141.5(3)
C(1)-Ir(1)-C(5)-C(6)	-58.5(3)
C(8)-Ir(1)-C(5)-C(6)	-24.8(3)
C(4)-Ir(1)-C(5)-C(6)	-123.4(4)
P(1)-Ir(1)-C(5)-C(6)	49.5(4)
C(4)-C(5)-C(6)-C(7)	-45.7(6)
Ir(1)-C(5)-C(6)-C(7)	37.6(4)
C(5)-C(6)-C(7)-C(8)	-31.1(5)
C(2)-C(1)-C(8)-C(7)	-2.7(6)
Ir(1)-C(1)-C(8)-C(7)	-104.2(4)
C(2)-C(1)-C(8)-Ir(1)	101.6(4)
C(6)-C(7)-C(8)-C(1)	90.3(5)
C(6)-C(7)-C(8)-Ir(1)	8.9(5)
C(9)-Ir(1)-C(8)-C(1)	-161.5(4)
C(5)-Ir(1)-C(8)-C(1)	-112.1(2)
C(4)-Ir(1)-C(8)-C(1)	-75.9(2)
P(1)-Ir(1)-C(8)-C(1)	92.9(2)
C(9)-Ir(1)-C(8)-C(7)	-40.7(6)
C(1)-Ir(1)-C(8)-C(7)	120.8(4)
C(5)-Ir(1)-C(8)-C(7)	8.7(3)
C(4)-Ir(1)-C(8)-C(7)	44.9(3)
P(1)-Ir(1)-C(8)-C(7)	-146.3(3)
C(11)-N(2)-C(9)-N(1)	-0.9(4)
C(18)-N(2)-C(9)-N(1)	-176.9(3)
C(11)-N(2)-C(9)-Ir(1)	175.6(3)
C(18)-N(2)-C(9)-Ir(1)	-0.4(5)
C(10)-N(1)-C(9)-N(2)	1.0(4)

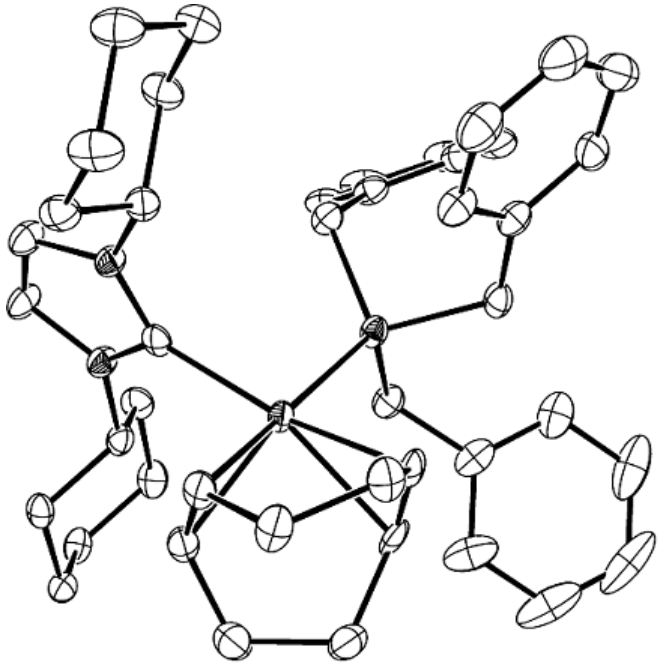
C(12)-N(1)-C(9)-N(2)	179.6(3)
C(10)-N(1)-C(9)-Ir(1)	-175.5(3)
C(12)-N(1)-C(9)-Ir(1)	3.1(5)
C(1)-Ir(1)-C(9)-N(2)	-168.0(3)
C(5)-Ir(1)-C(9)-N(2)	-69.7(3)
C(8)-Ir(1)-C(9)-N(2)	-21.3(7)
C(4)-Ir(1)-C(9)-N(2)	-106.2(3)
P(1)-Ir(1)-C(9)-N(2)	84.2(3)
C(1)-Ir(1)-C(9)-N(1)	7.7(6)
C(5)-Ir(1)-C(9)-N(1)	106.0(3)
C(8)-Ir(1)-C(9)-N(1)	154.4(4)
C(4)-Ir(1)-C(9)-N(1)	69.5(3)
P(1)-Ir(1)-C(9)-N(1)	-100.1(3)
C(9)-N(1)-C(10)-C(11)	-0.6(4)
C(12)-N(1)-C(10)-C(11)	-179.3(3)
N(1)-C(10)-C(11)-N(2)	0.0(5)
C(9)-N(2)-C(11)-C(10)	0.6(5)
C(18)-N(2)-C(11)-C(10)	176.6(3)
C(9)-N(1)-C(12)-C(17)	-115.8(4)
C(10)-N(1)-C(12)-C(17)	62.6(5)
C(9)-N(1)-C(12)-C(13)	120.7(4)
C(10)-N(1)-C(12)-C(13)	-60.9(5)
N(1)-C(12)-C(13)-C(14)	179.6(3)
C(17)-C(12)-C(13)-C(14)	55.9(5)
C(12)-C(13)-C(14)-C(15)	-54.8(5)
C(13)-C(14)-C(15)-C(16)	54.3(5)
C(14)-C(15)-C(16)-C(17)	-56.0(5)
C(15)-C(16)-C(17)-C(12)	57.9(5)
N(1)-C(12)-C(17)-C(16)	178.3(3)
C(13)-C(12)-C(17)-C(16)	-57.5(4)
C(9)-N(2)-C(18)-C(23)	116.4(4)
C(11)-N(2)-C(18)-C(23)	-59.1(5)
C(9)-N(2)-C(18)-C(19)	-119.3(4)
C(11)-N(2)-C(18)-C(19)	65.2(5)
N(2)-C(18)-C(19)-C(20)	-179.2(3)
C(23)-C(18)-C(19)-C(20)	-54.8(4)
C(18)-C(19)-C(20)-C(21)	54.6(4)
C(19)-C(20)-C(21)-C(22)	-57.0(4)
C(20)-C(21)-C(22)-C(23)	59.1(4)
C(21)-C(22)-C(23)-C(18)	-59.5(4)
N(2)-C(18)-C(23)-C(22)	-178.0(3)
C(19)-C(18)-C(23)-C(22)	57.5(4)
C(31)-P(1)-C(24)-C(25)	60.5(3)
C(38)-P(1)-C(24)-C(25)	167.0(3)
Ir(1)-P(1)-C(24)-C(25)	-70.1(3)
P(1)-C(24)-C(25)-C(26)	40.3(5)
P(1)-C(24)-C(25)-C(30)	-142.5(3)
C(30)-C(25)-C(26)-C(27)	-2.0(6)
C(24)-C(25)-C(26)-C(27)	175.3(4)
C(25)-C(26)-C(27)-C(28)	1.3(7)
C(26)-C(27)-C(28)-C(29)	0.1(7)
C(27)-C(28)-C(29)-C(30)	-0.8(7)

C(28)-C(29)-C(30)-C(25)	0.2(6)
C(26)-C(25)-C(30)-C(29)	1.2(6)
C(24)-C(25)-C(30)-C(29)	-176.2(4)
C(24)-P(1)-C(31)-C(32)	68.1(3)
C(38)-P(1)-C(31)-C(32)	-39.6(3)
Ir(1)-P(1)-C(31)-C(32)	-162.1(2)
P(1)-C(31)-C(32)-C(37)	105.1(4)
P(1)-C(31)-C(32)-C(33)	-71.4(5)
C(37)-C(32)-C(33)-C(34)	-2.6(6)
C(31)-C(32)-C(33)-C(34)	174.0(4)
C(32)-C(33)-C(34)-C(35)	2.0(7)
C(33)-C(34)-C(35)-C(36)	0.1(7)
C(34)-C(35)-C(36)-C(37)	-1.5(7)
C(33)-C(32)-C(37)-C(36)	1.2(6)
C(31)-C(32)-C(37)-C(36)	-175.4(4)
C(35)-C(36)-C(37)-C(32)	0.8(7)
C(24)-P(1)-C(38)-C(39A)	46.7(8)
C(31)-P(1)-C(38)-C(39A)	153.5(8)
Ir(1)-P(1)-C(38)-C(39A)	-79.6(8)
C(24)-P(1)-C(38)-C(39)	30.4(4)
C(31)-P(1)-C(38)-C(39)	137.2(4)
Ir(1)-P(1)-C(38)-C(39)	-95.9(4)
C(39A)-C(38)-C(39)-C(44)	-4(4)
P(1)-C(38)-C(39)-C(44)	107.7(6)
C(39A)-C(38)-C(39)-C(40)	172(5)
P(1)-C(38)-C(39)-C(40)	-76.5(7)
C(44)-C(39)-C(40)-C(41)	-1.9(10)
C(38)-C(39)-C(40)-C(41)	-177.6(7)
C(39)-C(40)-C(41)-C(42)	0.6(10)
C(40)-C(41)-C(42)-C(43)	1.5(12)
C(41)-C(42)-C(43)-C(44)	-2.5(13)
C(40)-C(39)-C(44)-C(43)	1.0(10)
C(38)-C(39)-C(44)-C(43)	176.8(8)
C(42)-C(43)-C(44)-C(39)	1.2(11)
C(1S)#1-O(1S)-C(1S)-C(2S)	168.5(13)
C(39)-C(38)-C(39A)-C(40A)	-3(4)
P(1)-C(38)-C(39A)-C(40A)	-80.2(12)
C(39)-C(38)-C(39A)-C(44A)	174(5)
P(1)-C(38)-C(39A)-C(44A)	97.4(11)
C(44A)-C(39A)-C(40A)-C(41A)	0.0
C(38)-C(39A)-C(40A)-C(41A)	177.6(18)
C(39A)-C(40A)-C(41A)-C(42A)	0.0
C(40A)-C(41A)-C(42A)-C(43A)	0.0
C(41A)-C(42A)-C(43A)-C(44A)	0.0
C(42A)-C(43A)-C(44A)-C(39A)	0.0
C(40A)-C(39A)-C(44A)-C(43A)	0.0
C(38)-C(39A)-C(44A)-C(43A)	-177.6(18)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2





Both structures emit hydrogen atoms and PF_6 anion.

8.3 Crystal data for 136

Table 1. Crystal data and structure refinement for kerrcochirfmonop.

Identification code	kerrcochirfmonop	
Empirical formula	C31 H47 F6 Ir N2 P2	
Formula weight	815.85	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 13.0899(5) Å	α= 90°.
	b = 15.1282(5) Å	β= 110.183(3)°.
	c = 17.3520(6) Å	γ = 90°.
Volume	3225.2(2) $Å^3$	
Z	4	
Density (calculated)	1.680 Mg/m^3	
Absorption coefficient	4.298 mm^{-1}	
F(000)	1632	
Crystal size	0.31 x 0.13 x 0.06 mm^3	
Theta range for data collection	2.97 to 28.88°.	
Index ranges	-17<=h<=17, -17<=k<=19, -23<=l<=22	
Reflections collected	18193	
Independent reflections	7418 [R(int) = 0.0583]	
Completeness to theta = 26.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.70870	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7418 / 64 / 381	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.0723	
R indices (all data)	R1 = 0.0780, wR2 = 0.0848	
Largest diff. peak and hole	1.538 and -1.309 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Ir(1)	3898(1)	1148(1)	1863(1)	15(1)
P(1)	2457(1)	1844(1)	903(1)	20(1)
P(2)	6288(2)	6279(1)	3775(1)	33(1)
F(1)	6178(3)	6204(3)	4659(2)	63(1)
F(2)	5821(4)	7240(3)	3679(3)	82(2)

F(3)	7492(3)	6652(3)	4183(3)	60(1)
F(4)	6418(4)	6322(3)	2900(3)	76(2)
F(5)	5076(3)	5894(3)	3374(2)	56(1)
F(6)	6757(4)	5294(2)	3882(3)	62(1)
N(1)	4621(4)	3030(3)	2586(3)	16(1)
N(2)	3720(4)	2325(3)	3222(3)	17(1)
C(1)	4136(4)	2241(4)	2605(3)	16(1)
C(2)	4497(5)	3596(4)	3172(3)	21(1)
C(3)	3927(5)	3166(4)	3560(3)	20(1)
C(4)	5340(4)	3201(3)	2103(3)	15(1)
C(5)	5000(5)	4037(4)	1583(3)	24(1)
C(6)	5759(5)	4189(4)	1099(3)	29(2)
C(7)	6930(5)	4248(4)	1664(4)	26(1)
C(8)	7265(5)	3424(4)	2193(4)	27(1)
C(9)	6505(4)	3268(4)	2673(3)	19(1)
C(10)	3177(4)	1615(4)	3510(3)	18(1)
C(11)	2053(5)	1875(4)	3499(4)	27(2)
C(12)	1514(5)	1090(4)	3755(4)	34(2)
C(13)	2209(6)	765(4)	4609(4)	35(2)
C(14)	3336(5)	527(4)	4630(4)	34(2)
C(15)	3886(5)	1306(4)	4360(3)	28(2)
C(16)	5820(5)	300(4)	1572(4)	29(1)
C(17)	5600(5)	758(4)	2275(3)	23(1)
C(18)	5163(5)	385(4)	2829(3)	22(1)
C(19)	4836(5)	-572(4)	2836(4)	26(1)
C(20)	3646(5)	-740(4)	2312(4)	29(1)
C(21)	3237(5)	-165(3)	1552(3)	22(1)
C(22)	3804(5)	13(3)	1017(3)	23(1)
C(23)	4907(5)	-355(4)	1110(4)	30(1)
C(24)	1344(5)	1173(4)	259(3)	29(1)
C(25)	1738(5)	2672(4)	1272(4)	31(2)
C(26)	2924(5)	2434(3)	164(3)	20(1)
C(27)	3839(5)	2143(4)	1(4)	25(1)
C(28)	4193(6)	2564(4)	-568(4)	33(2)
C(29)	3627(5)	3288(4)	-981(4)	31(2)
C(30)	2753(5)	3603(4)	-820(4)	31(2)
C(31)	2382(5)	3170(4)	-259(4)	28(2)

Table 3. Bond lengths [Å] and angles [°] for kerrcochirfmonop.

Ir(1)-C(1)	2.053(5)
Ir(1)-C(21)	2.159(5)
Ir(1)-C(17)	2.173(6)
Ir(1)-C(18)	2.229(5)
Ir(1)-C(22)	2.235(5)
Ir(1)-P(1)	2.2962(15)
P(1)-C(24)	1.811(6)

P(1)-C(25)	1.811(6)
P(1)-C(26)	1.831(6)
P(2)-F(2)	1.562(4)
P(2)-F(4)	1.586(4)
P(2)-F(3)	1.592(4)
P(2)-F(1)	1.593(4)
P(2)-F(6)	1.599(4)
P(2)-F(5)	1.606(4)
N(1)-C(1)	1.358(6)
N(1)-C(2)	1.380(6)
N(1)-C(4)	1.483(6)
N(2)-C(1)	1.363(6)
N(2)-C(3)	1.388(6)
N(2)-C(10)	1.467(6)
C(2)-C(3)	1.334(7)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(4)-C(9)	1.508(7)
C(4)-C(5)	1.527(7)
C(4)-H(4)	1.0000
C(5)-C(6)	1.524(8)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.510(8)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.520(7)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.521(7)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.516(8)
C(10)-C(15)	1.520(7)
C(10)-H(10)	1.0000
C(11)-C(12)	1.524(7)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.527(8)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.507(9)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.536(8)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.514(8)

C(16)-C(23)	1.546(8)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.397(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.510(7)
C(18)-H(18)	0.9500
C(19)-C(20)	1.530(8)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.515(8)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.401(8)
C(21)-H(21)	0.9500
C(22)-C(23)	1.503(8)
C(22)-H(22)	0.9500
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-C(31)	1.386(7)
C(26)-C(27)	1.395(8)
C(27)-C(28)	1.383(8)
C(27)-H(27)	0.9500
C(28)-C(29)	1.377(8)
C(28)-H(28)	0.9500
C(29)-C(30)	1.354(8)
C(29)-H(29)	0.9500
C(30)-C(31)	1.394(8)
C(30)-H(30)	0.9500
C(31)-H(31)	0.9500

C(1)-Ir(1)-C(21)	149.1(2)
C(1)-Ir(1)-C(17)	95.5(2)
C(21)-Ir(1)-C(17)	96.3(2)
C(1)-Ir(1)-C(18)	91.9(2)
C(21)-Ir(1)-C(18)	80.9(2)
C(17)-Ir(1)-C(18)	37.0(2)
C(1)-Ir(1)-C(22)	173.3(2)
C(21)-Ir(1)-C(22)	37.1(2)
C(17)-Ir(1)-C(22)	79.9(2)
C(18)-Ir(1)-C(22)	87.4(2)
C(1)-Ir(1)-P(1)	89.71(15)
C(21)-Ir(1)-P(1)	94.72(16)
C(17)-Ir(1)-P(1)	148.81(15)
C(18)-Ir(1)-P(1)	173.73(15)
C(22)-Ir(1)-P(1)	91.75(16)

C(24)-P(1)-C(25)	101.6(3)
C(24)-P(1)-C(26)	103.5(3)
C(25)-P(1)-C(26)	104.4(3)
C(24)-P(1)-Ir(1)	118.4(2)
C(25)-P(1)-Ir(1)	117.2(2)
C(26)-P(1)-Ir(1)	110.01(19)
F(2)-P(2)-F(4)	91.6(3)
F(2)-P(2)-F(3)	90.5(3)
F(4)-P(2)-F(3)	89.7(3)
F(2)-P(2)-F(1)	90.4(3)
F(4)-P(2)-F(1)	178.0(3)
F(3)-P(2)-F(1)	90.1(2)
F(2)-P(2)-F(6)	179.2(3)
F(4)-P(2)-F(6)	89.1(2)
F(3)-P(2)-F(6)	89.8(2)
F(1)-P(2)-F(6)	88.9(2)
F(2)-P(2)-F(5)	90.0(3)
F(4)-P(2)-F(5)	90.9(3)
F(3)-P(2)-F(5)	179.2(3)
F(1)-P(2)-F(5)	89.3(2)
F(6)-P(2)-F(5)	89.6(2)
C(1)-N(1)-C(2)	110.6(4)
C(1)-N(1)-C(4)	124.1(4)
C(2)-N(1)-C(4)	124.5(4)
C(1)-N(2)-C(3)	110.1(4)
C(1)-N(2)-C(10)	124.9(4)
C(3)-N(2)-C(10)	125.0(4)
N(1)-C(1)-N(2)	104.7(4)
N(1)-C(1)-Ir(1)	131.6(4)
N(2)-C(1)-Ir(1)	123.5(4)
C(3)-C(2)-N(1)	107.3(5)
C(3)-C(2)-H(2)	126.3
N(1)-C(2)-H(2)	126.3
C(2)-C(3)-N(2)	107.2(5)
C(2)-C(3)-H(3)	126.4
N(2)-C(3)-H(3)	126.4
N(1)-C(4)-C(9)	109.6(4)
N(1)-C(4)-C(5)	111.4(4)
C(9)-C(4)-C(5)	110.8(4)
N(1)-C(4)-H(4)	108.3
C(9)-C(4)-H(4)	108.3
C(5)-C(4)-H(4)	108.3
C(6)-C(5)-C(4)	109.7(5)
C(6)-C(5)-H(5A)	109.7
C(4)-C(5)-H(5A)	109.7
C(6)-C(5)-H(5B)	109.7
C(4)-C(5)-H(5B)	109.7
H(5A)-C(5)-H(5B)	108.2
C(7)-C(6)-C(5)	111.1(5)
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6B)	109.4

C(5)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(6)-C(7)-C(8)	111.1(5)
C(6)-C(7)-H(7A)	109.4
C(8)-C(7)-H(7A)	109.4
C(6)-C(7)-H(7B)	109.4
C(8)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
C(7)-C(8)-C(9)	110.6(5)
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
C(9)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(4)-C(9)-C(8)	110.8(5)
C(4)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	108.1
N(2)-C(10)-C(11)	112.9(4)
N(2)-C(10)-C(15)	110.5(5)
C(11)-C(10)-C(15)	110.9(5)
N(2)-C(10)-H(10)	107.4
C(11)-C(10)-H(10)	107.4
C(15)-C(10)-H(10)	107.4
C(10)-C(11)-C(12)	109.9(5)
C(10)-C(11)-H(11A)	109.7
C(12)-C(11)-H(11A)	109.7
C(10)-C(11)-H(11B)	109.7
C(12)-C(11)-H(11B)	109.7
H(11A)-C(11)-H(11B)	108.2
C(11)-C(12)-C(13)	110.7(5)
C(11)-C(12)-H(12A)	109.5
C(13)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
C(13)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	108.1
C(14)-C(13)-C(12)	110.6(5)
C(14)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.1
C(13)-C(14)-C(15)	111.6(5)
C(13)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14B)	109.3
C(15)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
C(10)-C(15)-C(14)	109.8(5)
C(10)-C(15)-H(15A)	109.7

C(14)-C(15)-H(15A)	109.7
C(10)-C(15)-H(15B)	109.7
C(14)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
C(17)-C(16)-C(23)	112.5(5)
C(17)-C(16)-H(16A)	109.1
C(23)-C(16)-H(16A)	109.1
C(17)-C(16)-H(16B)	109.1
C(23)-C(16)-H(16B)	109.1
H(16A)-C(16)-H(16B)	107.8
C(18)-C(17)-C(16)	127.3(5)
C(18)-C(17)-Ir(1)	73.7(3)
C(16)-C(17)-Ir(1)	108.5(4)
C(18)-C(17)-H(17)	116.3
C(16)-C(17)-H(17)	116.3
Ir(1)-C(17)-H(17)	87.6
C(17)-C(18)-C(19)	125.2(5)
C(17)-C(18)-Ir(1)	69.3(3)
C(19)-C(18)-Ir(1)	111.3(4)
C(17)-C(18)-H(18)	117.4
C(19)-C(18)-H(18)	117.4
Ir(1)-C(18)-H(18)	89.3
C(18)-C(19)-C(20)	112.9(5)
C(18)-C(19)-H(19A)	109.0
C(20)-C(19)-H(19A)	109.0
C(18)-C(19)-H(19B)	109.0
C(20)-C(19)-H(19B)	109.0
H(19A)-C(19)-H(19B)	107.8
C(21)-C(20)-C(19)	113.8(5)
C(21)-C(20)-H(20A)	108.8
C(19)-C(20)-H(20A)	108.8
C(21)-C(20)-H(20B)	108.8
C(19)-C(20)-H(20B)	108.8
H(20A)-C(20)-H(20B)	107.7
C(22)-C(21)-C(20)	125.3(6)
C(22)-C(21)-Ir(1)	74.4(3)
C(20)-C(21)-Ir(1)	108.7(4)
C(22)-C(21)-H(21)	117.4
C(20)-C(21)-H(21)	117.4
Ir(1)-C(21)-H(21)	86.8
C(21)-C(22)-C(23)	124.5(5)
C(21)-C(22)-Ir(1)	68.5(3)
C(23)-C(22)-Ir(1)	112.4(4)
C(21)-C(22)-H(22)	117.7
C(23)-C(22)-H(22)	117.7
Ir(1)-C(22)-H(22)	89.2
C(22)-C(23)-C(16)	111.1(5)
C(22)-C(23)-H(23A)	109.4
C(16)-C(23)-H(23A)	109.4
C(22)-C(23)-H(23B)	109.4
C(16)-C(23)-H(23B)	109.4
H(23A)-C(23)-H(23B)	108.0

P(1)-C(24)-H(24A)	109.5
P(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
P(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
P(1)-C(25)-H(25A)	109.5
P(1)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
P(1)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(31)-C(26)-C(27)	117.7(5)
C(31)-C(26)-P(1)	121.9(5)
C(27)-C(26)-P(1)	120.4(4)
C(28)-C(27)-C(26)	121.5(6)
C(28)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3
C(29)-C(28)-C(27)	119.1(6)
C(29)-C(28)-H(28)	120.5
C(27)-C(28)-H(28)	120.5
C(30)-C(29)-C(28)	120.9(6)
C(30)-C(29)-H(29)	119.5
C(28)-C(29)-H(29)	119.5
C(29)-C(30)-C(31)	120.1(6)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(26)-C(31)-C(30)	120.6(6)
C(26)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	16(1)	13(1)	14(1)	-1(1)	3(1)	-1(1)
P(1)	20(1)	22(1)	15(1)	-2(1)	1(1)	4(1)
P(2)	44(1)	31(1)	30(1)	-2(1)	20(1)	-4(1)
F(1)	60(3)	102(4)	38(2)	-22(2)	29(2)	-22(3)
F(2)	68(4)	35(3)	137(5)	-1(3)	29(4)	16(2)
F(3)	46(3)	66(3)	76(3)	-7(3)	31(3)	-14(2)
F(4)	118(4)	87(4)	41(3)	10(2)	50(3)	-8(3)
F(5)	54(3)	69(3)	43(3)	-14(2)	13(2)	-23(2)
F(6)	88(4)	33(2)	73(3)	5(2)	39(3)	8(2)

N(1)	16(3)	11(2)	20(2)	-2(2)	4(2)	-4(2)
N(2)	16(3)	19(3)	16(2)	-3(2)	5(2)	-4(2)
C(1)	14(3)	18(3)	11(3)	1(2)	-3(2)	4(2)
C(2)	22(3)	13(3)	22(3)	-3(2)	2(3)	0(2)
C(3)	27(4)	17(3)	16(3)	-6(2)	7(3)	0(3)
C(4)	16(3)	15(3)	16(3)	-1(2)	7(2)	-2(2)
C(5)	20(3)	23(3)	20(3)	4(3)	-4(3)	2(3)
C(6)	37(4)	32(4)	18(3)	6(3)	8(3)	-6(3)
C(7)	27(4)	24(3)	29(3)	-3(3)	12(3)	-6(3)
C(8)	23(3)	23(3)	37(4)	0(3)	12(3)	-2(3)
C(9)	16(3)	15(3)	23(3)	2(2)	3(3)	3(2)
C(10)	22(3)	13(3)	20(3)	1(2)	9(3)	-2(3)
C(11)	26(4)	30(4)	24(3)	1(3)	6(3)	-4(3)
C(12)	26(4)	37(4)	39(4)	11(3)	14(3)	-7(3)
C(13)	49(5)	26(4)	35(4)	2(3)	23(4)	-7(3)
C(14)	49(5)	27(4)	22(3)	8(3)	9(3)	-3(3)
C(15)	29(4)	31(4)	18(3)	1(3)	3(3)	0(3)
C(16)	29(3)	28(3)	27(3)	8(3)	9(3)	7(3)
C(17)	20(3)	15(3)	28(3)	4(2)	2(2)	1(2)
C(18)	25(3)	14(3)	22(3)	1(2)	2(2)	5(2)
C(19)	36(3)	18(3)	25(3)	10(3)	12(3)	4(3)
C(20)	38(4)	14(3)	34(3)	0(2)	12(3)	-9(3)
C(21)	27(3)	10(3)	25(3)	-2(2)	2(2)	-3(2)
C(22)	37(3)	7(3)	21(3)	-6(2)	7(3)	4(2)
C(23)	42(4)	26(3)	21(3)	1(2)	13(3)	12(3)
C(24)	16(3)	41(4)	24(3)	0(3)	-1(3)	2(3)
C(25)	29(4)	39(4)	23(3)	0(3)	6(3)	14(3)
C(26)	26(4)	14(3)	12(3)	-4(2)	-2(3)	1(3)
C(27)	38(4)	12(3)	27(3)	-3(3)	13(3)	3(3)
C(28)	40(4)	34(4)	26(3)	-7(3)	12(3)	2(3)
C(29)	46(5)	20(4)	21(3)	-4(3)	4(3)	-17(3)
C(30)	37(4)	22(4)	28(3)	7(3)	3(3)	6(3)
C(31)	17(3)	31(4)	30(3)	4(3)	1(3)	1(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for kerrcochirfmonop.

	x	y	z	U(eq)
H(2)	4768	4183	3279	25
H(3)	3705	3393	3988	24
H(4)	5281	2689	1726	19
H(5A)	4242	3974	1201	29
H(5B)	5031	4551	1944	29
H(6A)	5680	3697	707	35
H(6B)	5553	4744	780	35

H(7A)	7023	4774	2021	31
H(7B)	7407	4320	1333	31
H(8A)	8020	3494	2579	32
H(8B)	7245	2906	1839	32
H(9A)	6714	2715	2994	23
H(9B)	6576	3761	3063	23
H(10)	3086	1104	3127	22
H(11A)	1602	2069	2940	32
H(11B)	2113	2374	3881	32
H(12A)	1415	604	3353	40
H(12B)	787	1266	3758	40
H(13A)	2256	1233	5018	42
H(13B)	1862	240	4755	42
H(14A)	3292	17	4263	40
H(14B)	3785	349	5195	40
H(15A)	3999	1798	4756	33
H(15B)	4607	1119	4349	33
H(16A)	6518	-24	1789	34
H(16B)	5894	751	1181	34
H(17)	5780	1368	2347	28
H(18)	5063	763	3234	26
H(19A)	4955	-753	3408	31
H(19B)	5309	-942	2629	31
H(20A)	3563	-1369	2141	35
H(20B)	3187	-637	2652	35
H(21)	2539	97	1429	27
H(22)	3469	392	563	27
H(23A)	4946	-478	561	35
H(23B)	5016	-920	1417	35
H(24A)	989	875	600	44
H(24B)	1626	730	-28	44
H(24C)	815	1551	-144	44
H(25A)	1197	2964	803	47
H(25B)	2257	3112	1599	47
H(25C)	1372	2389	1613	47
H(27)	4229	1643	287	30
H(28)	4819	2358	-672	40
H(29)	3852	3570	-1385	37
H(30)	2393	4121	-1091	37
H(31)	1751	3381	-165	33

Table 6. Torsion angles [°] for kerrcochirfmonop.

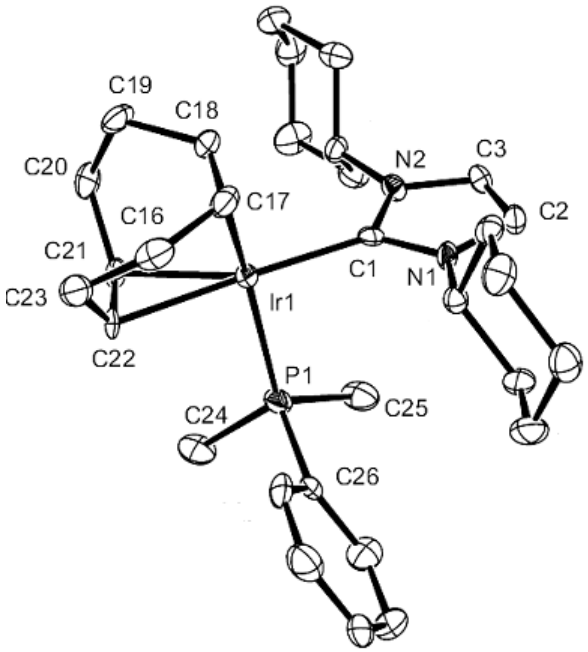
C(1)-Ir(1)-P(1)-C(24)	-149.4(3)
C(21)-Ir(1)-P(1)-C(24)	0.1(3)
C(17)-Ir(1)-P(1)-C(24)	110.5(4)
C(18)-Ir(1)-P(1)-C(24)	-44.8(14)

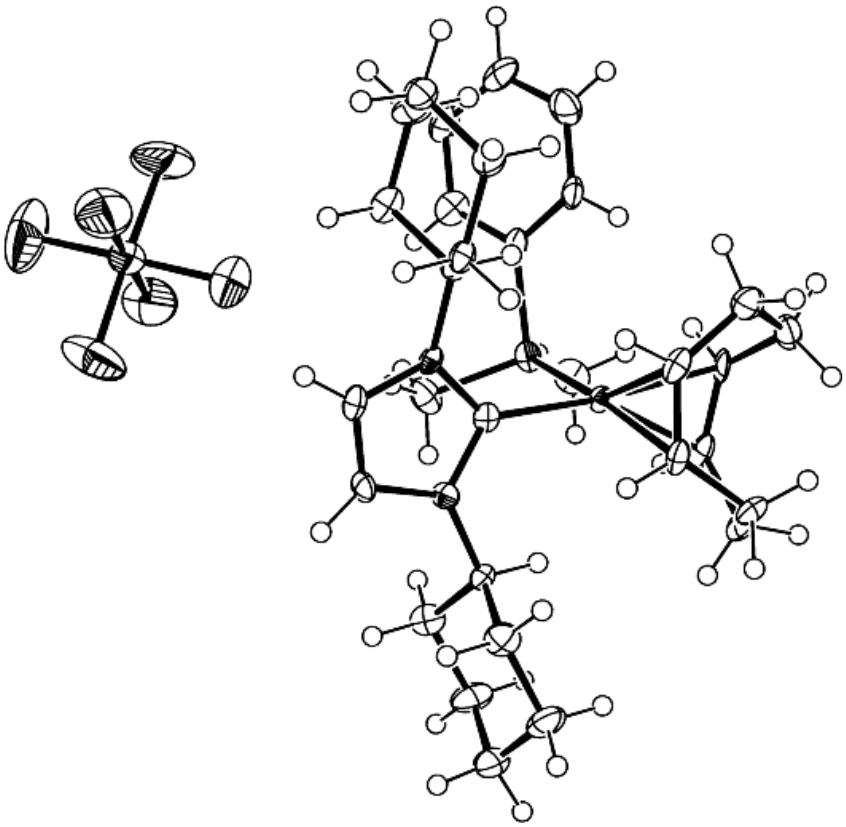
C(22)-Ir(1)-P(1)-C(24)	37.2(3)
C(1)-Ir(1)-P(1)-C(25)	-27.1(3)
C(21)-Ir(1)-P(1)-C(25)	122.4(3)
C(17)-Ir(1)-P(1)-C(25)	-127.2(4)
C(18)-Ir(1)-P(1)-C(25)	77.5(14)
C(22)-Ir(1)-P(1)-C(25)	159.4(3)
C(1)-Ir(1)-P(1)-C(26)	92.0(2)
C(21)-Ir(1)-P(1)-C(26)	-118.6(2)
C(17)-Ir(1)-P(1)-C(26)	-8.2(4)
C(18)-Ir(1)-P(1)-C(26)	-163.4(14)
C(22)-Ir(1)-P(1)-C(26)	-81.5(2)
C(2)-N(1)-C(1)-N(2)	-0.7(6)
C(4)-N(1)-C(1)-N(2)	169.6(4)
C(2)-N(1)-C(1)-Ir(1)	174.4(4)
C(4)-N(1)-C(1)-Ir(1)	-15.2(8)
C(3)-N(2)-C(1)-N(1)	1.5(6)
C(10)-N(2)-C(1)-N(1)	-175.9(5)
C(3)-N(2)-C(1)-Ir(1)	-174.2(4)
C(10)-N(2)-C(1)-Ir(1)	8.5(7)
C(21)-Ir(1)-C(1)-N(1)	-177.7(4)
C(17)-Ir(1)-C(1)-N(1)	70.3(5)
C(18)-Ir(1)-C(1)-N(1)	107.1(5)
C(22)-Ir(1)-C(1)-N(1)	24(2)
P(1)-Ir(1)-C(1)-N(1)	-78.9(5)
C(21)-Ir(1)-C(1)-N(2)	-3.3(7)
C(17)-Ir(1)-C(1)-N(2)	-115.4(4)
C(18)-Ir(1)-C(1)-N(2)	-78.5(4)
C(22)-Ir(1)-C(1)-N(2)	-161.9(16)
P(1)-Ir(1)-C(1)-N(2)	95.4(4)
C(1)-N(1)-C(2)-C(3)	-0.3(6)
C(4)-N(1)-C(2)-C(3)	-170.6(5)
N(1)-C(2)-C(3)-N(2)	1.2(6)
C(1)-N(2)-C(3)-C(2)	-1.7(6)
C(10)-N(2)-C(3)-C(2)	175.6(5)
C(1)-N(1)-C(4)-C(9)	-107.1(5)
C(2)-N(1)-C(4)-C(9)	61.9(6)
C(1)-N(1)-C(4)-C(5)	129.8(5)
C(2)-N(1)-C(4)-C(5)	-61.2(7)
N(1)-C(4)-C(5)-C(6)	179.9(4)
C(9)-C(4)-C(5)-C(6)	57.5(6)
C(4)-C(5)-C(6)-C(7)	-56.9(6)
C(5)-C(6)-C(7)-C(8)	56.6(6)
C(6)-C(7)-C(8)-C(9)	-55.9(6)
N(1)-C(4)-C(9)-C(8)	178.8(4)
C(5)-C(4)-C(9)-C(8)	-57.8(6)
C(7)-C(8)-C(9)-C(4)	56.6(6)
C(1)-N(2)-C(10)-C(11)	-125.7(6)
C(3)-N(2)-C(10)-C(11)	57.3(7)
C(1)-N(2)-C(10)-C(15)	109.5(6)
C(3)-N(2)-C(10)-C(15)	-67.5(7)
N(2)-C(10)-C(11)-C(12)	176.5(5)
C(15)-C(10)-C(11)-C(12)	-58.8(6)

C(10)-C(11)-C(12)-C(13)	58.1(7)
C(11)-C(12)-C(13)-C(14)	-56.9(7)
C(12)-C(13)-C(14)-C(15)	56.0(7)
N(2)-C(10)-C(15)-C(14)	-176.7(4)
C(11)-C(10)-C(15)-C(14)	57.4(6)
C(13)-C(14)-C(15)-C(10)	-56.1(7)
C(23)-C(16)-C(17)-C(18)	40.1(8)
C(23)-C(16)-C(17)-Ir(1)	-43.1(6)
C(1)-Ir(1)-C(17)-C(18)	85.8(4)
C(21)-Ir(1)-C(17)-C(18)	-65.7(4)
C(22)-Ir(1)-C(17)-C(18)	-99.1(4)
P(1)-Ir(1)-C(17)-C(18)	-175.6(3)
C(1)-Ir(1)-C(17)-C(16)	-149.6(4)
C(21)-Ir(1)-C(17)-C(16)	59.0(4)
C(18)-Ir(1)-C(17)-C(16)	124.6(5)
C(22)-Ir(1)-C(17)-C(16)	25.5(4)
P(1)-Ir(1)-C(17)-C(16)	-51.0(5)
C(16)-C(17)-C(18)-C(19)	1.0(9)
Ir(1)-C(17)-C(18)-C(19)	102.1(5)
C(16)-C(17)-C(18)-Ir(1)	-101.1(6)
C(1)-Ir(1)-C(18)-C(17)	-96.7(4)
C(21)-Ir(1)-C(18)-C(17)	113.5(4)
C(22)-Ir(1)-C(18)-C(17)	76.7(4)
P(1)-Ir(1)-C(18)-C(17)	158.9(12)
C(1)-Ir(1)-C(18)-C(19)	142.4(4)
C(21)-Ir(1)-C(18)-C(19)	-7.5(4)
C(17)-Ir(1)-C(18)-C(19)	-121.0(6)
C(22)-Ir(1)-C(18)-C(19)	-44.3(4)
P(1)-Ir(1)-C(18)-C(19)	37.9(16)
C(17)-C(18)-C(19)-C(20)	-90.7(7)
Ir(1)-C(18)-C(19)-C(20)	-11.6(6)
C(18)-C(19)-C(20)-C(21)	34.2(7)
C(19)-C(20)-C(21)-C(22)	44.3(8)
C(19)-C(20)-C(21)-Ir(1)	-39.4(6)
C(1)-Ir(1)-C(21)-C(22)	-176.0(4)
C(17)-Ir(1)-C(21)-C(22)	-64.1(4)
C(18)-Ir(1)-C(21)-C(22)	-97.8(4)
P(1)-Ir(1)-C(21)-C(22)	86.7(3)
C(1)-Ir(1)-C(21)-C(20)	-53.4(6)
C(17)-Ir(1)-C(21)-C(20)	58.5(4)
C(18)-Ir(1)-C(21)-C(20)	24.8(4)
C(22)-Ir(1)-C(21)-C(20)	122.6(6)
P(1)-Ir(1)-C(21)-C(20)	-150.8(4)
C(20)-C(21)-C(22)-C(23)	0.9(9)
Ir(1)-C(21)-C(22)-C(23)	103.0(5)
C(20)-C(21)-C(22)-Ir(1)	-102.1(5)
C(1)-Ir(1)-C(22)-C(21)	161.9(16)
C(17)-Ir(1)-C(22)-C(21)	114.7(4)
C(18)-Ir(1)-C(22)-C(21)	78.3(4)
P(1)-Ir(1)-C(22)-C(21)	-95.5(3)
C(1)-Ir(1)-C(22)-C(23)	42.2(19)
C(21)-Ir(1)-C(22)-C(23)	-119.8(6)

C(17)-Ir(1)-C(22)-C(23)	-5.0(4)
C(18)-Ir(1)-C(22)-C(23)	-41.5(4)
P(1)-Ir(1)-C(22)-C(23)	144.7(4)
C(21)-C(22)-C(23)-C(16)	-95.0(6)
Ir(1)-C(22)-C(23)-C(16)	-16.4(6)
C(17)-C(16)-C(23)-C(22)	39.7(7)
C(24)-P(1)-C(26)-C(31)	79.1(5)
C(25)-P(1)-C(26)-C(31)	-26.9(5)
Ir(1)-P(1)-C(26)-C(31)	-153.5(4)
C(24)-P(1)-C(26)-C(27)	-99.9(5)
C(25)-P(1)-C(26)-C(27)	154.2(5)
Ir(1)-P(1)-C(26)-C(27)	27.5(5)
C(31)-C(26)-C(27)-C(28)	-0.6(9)
P(1)-C(26)-C(27)-C(28)	178.4(5)
C(26)-C(27)-C(28)-C(29)	0.0(9)
C(27)-C(28)-C(29)-C(30)	1.9(9)
C(28)-C(29)-C(30)-C(31)	-3.1(9)
C(27)-C(26)-C(31)-C(30)	-0.7(9)
P(1)-C(26)-C(31)-C(30)	-179.7(4)
C(29)-C(30)-C(31)-C(26)	2.5(9)

Symmetry transformations used to generate equivalent atoms:





View with PF_6 anion. Both structures omit hydrogen atoms.