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SUPPORTING INFORMATION

Iridium complexes of chiral diamines containing carbon and nitrogen stereocentres: synthesis, structure and evaluation as transfer hydrogenation catalysts

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Crystallographic data of complex 4 (mfmc1)

Table 1. Crystal data and structure refinement for mfmc1.

Identification code	mfmc1	
Empirical formula	C36 H51 B Cl7 F4 Ir N2	
Formula weight	1038.95	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 13.5451(7) Å	α= 90°.
	b = 17.3548(10) Å	β= 90°.
	c = 18.4163(10) Å	γ = 90°.
Volume	4329.2(4) Å^3	
Z	4	
Density (calculated)	1.594 Mg/m^3	
Absorption coefficient	3.561 mm^{-1}	
F(000)	2072	
Crystal size	0.1000 x 0.1000 x 0.1000 mm^3	
Theta range for data collection	1.87 to 25.36°.	
Index ranges	-16<=h<=14, -20<=k<=19, -22<=l<=18	
Reflections collected	28479	
Independent reflections	7939 [R(int) = 0.0423]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.7678	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7939 / 2 / 474	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0570	
R indices (all data)	R1 = 0.0306, wR2 = 0.0578	
Absolute structure parameter	-0.011(4)	
Largest diff. peak and hole	1.234 and -0.548 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mfmc1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	2967(1)	6458(1)	725(1)	15(1)
Cl(1)	4269(1)	7181(1)	139(1)	22(1)
N(1)	3714(2)	6472(2)	1773(2)	14(1)
C(1)	3960(3)	7291(2)	1986(2)	17(1)
C(2)	3007(4)	7754(2)	1872(2)	16(1)
N(2)	2648(3)	7632(2)	1108(2)	19(1)
C(3)	3208(3)	8597(2)	2045(2)	21(1)
C(4)	3543(4)	8706(2)	2834(2)	24(1)
C(5)	4468(4)	8215(3)	2990(3)	26(1)
C(6)	4296(4)	7373(2)	2770(3)	21(1)
C(7)	4526(3)	5880(3)	1869(2)	19(1)
C(8)	4682(3)	5660(2)	2663(2)	19(1)
C(9)	3893(4)	5514(2)	3127(3)	22(1)
C(10)	4037(4)	5327(3)	3842(3)	28(1)
C(11)	4982(4)	5249(3)	4115(3)	32(1)
C(12)	5777(4)	5363(3)	3667(3)	30(1)
C(13)	5633(4)	5579(3)	2947(3)	26(1)
C(14)	5467(4)	6113(3)	1466(3)	32(1)
C(15)	1630(3)	7978(3)	952(2)	18(1)
C(16)	1730(3)	8808(2)	682(3)	19(1)
C(17)	1196(3)	9415(3)	996(3)	22(1)
C(18)	1289(3)	10156(3)	731(3)	28(1)
C(19)	1916(4)	10309(3)	158(3)	32(1)
C(20)	2432(4)	9713(3)	-171(3)	30(1)
C(21)	2336(4)	8966(3)	88(3)	26(1)
C(22)	925(3)	7868(3)	1590(2)	22(1)
C(23)	2701(4)	8537(3)	3362(3)	38(1)
C(24)	5387(4)	8535(3)	2653(3)	34(1)
C(25)	2250(3)	5338(2)	852(2)	19(1)
C(26)	1551(3)	5884(2)	577(2)	19(1)
C(27)	1915(3)	6164(2)	-113(2)	19(1)
C(28)	2820(3)	5771(2)	-261(2)	19(1)
C(29)	3052(4)	5274(2)	330(2)	20(1)
C(30)	2139(4)	4858(3)	1519(2)	27(1)
C(31)	553(3)	6045(3)	904(3)	24(1)
C(32)	1376(3)	6677(3)	-650(3)	25(1)
C(33)	3411(4)	5841(3)	-941(2)	27(1)
C(34)	3886(4)	4719(3)	352(3)	26(1)
B(1)	1133(4)	6261(3)	3161(3)	29(1)
F(1)	526(2)	6904(2)	3190(2)	45(1)
F(2)	1646(3)	6179(2)	3801(2)	60(1)
F(3)	1801(2)	6351(2)	2594(1)	31(1)
F(4)	566(2)	5619(2)	3023(2)	55(1)
C(35)	5123(7)	7157(4)	5414(4)	77(2)
Cl(2)	3958(2)	7282(2)	5011(1)	126(1)
Cl(3)	5168(2)	6301(1)	5877(1)	77(1)
Cl(4)	6058(2)	7213(1)	4745(1)	98(1)
C(36)	8515(4)	6475(3)	2420(3)	41(1)
Cl(5)	7769(1)	6847(1)	3128(1)	56(1)
Cl(6)	8358(1)	6990(1)	1619(1)	47(1)
Cl(7)	8249(1)	5493(1)	2264(1)	47(1)

Table 3. Bond lengths [Å] and angles [°] for mfmc1.

Ir(1)-C(27)	2.161(4)
Ir(1)-C(26)	2.179(4)
Ir(1)-N(1)	2.179(3)
Ir(1)-C(28)	2.182(4)
Ir(1)-C(29)	2.182(4)
Ir(1)-C(25)	2.185(4)
Ir(1)-N(2)	2.199(4)
Ir(1)-Cl(1)	2.4187(11)
N(1)-C(1)	1.512(5)
N(1)-C(7)	1.515(5)
N(1)-H(1N)	0.978(5)
C(1)-C(6)	1.522(6)
C(1)-C(2)	1.534(6)
C(1)-H(1A)	1.0000
C(2)-N(2)	1.504(5)
C(2)-C(3)	1.521(6)
C(2)-H(2A)	1.0000
N(2)-C(15)	1.532(5)
N(2)-H(2N)	0.978(5)
C(3)-C(4)	1.535(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(23)	1.527(7)
C(4)-C(5)	1.541(7)
C(4)-H(4A)	1.0000
C(5)-C(24)	1.497(7)
C(5)-C(6)	1.534(6)
C(5)-H(5A)	1.0000
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.525(6)
C(7)-C(14)	1.529(7)
C(7)-H(7A)	1.0000
C(8)-C(9)	1.392(6)
C(8)-C(13)	1.398(7)
C(9)-C(10)	1.370(6)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.383(7)
C(10)-H(10A)	0.9500
C(11)-C(12)	1.371(7)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.391(7)
C(12)-H(12A)	0.9500
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(22)	1.527(6)
C(15)-C(16)	1.529(6)
C(15)-H(15A)	1.0000
C(16)-C(21)	1.394(6)
C(16)-C(17)	1.402(6)
C(17)-C(18)	1.383(6)
C(17)-H(17A)	0.9500
C(18)-C(19)	1.379(7)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.388(7)
C(19)-H(19A)	0.9500

C(20)-C(21)	1.387(7)
C(20)-H(20A)	0.9500
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.432(6)
C(25)-C(29)	1.455(6)
C(25)-C(30)	1.492(6)
C(26)-C(27)	1.447(6)
C(26)-C(31)	1.506(6)
C(27)-C(28)	1.429(6)
C(27)-C(32)	1.518(6)
C(28)-C(29)	1.424(6)
C(28)-C(33)	1.491(6)
C(29)-C(34)	1.485(6)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
B(1)-F(4)	1.377(7)
B(1)-F(2)	1.376(7)
B(1)-F(1)	1.387(6)
B(1)-F(3)	1.389(6)
C(35)-Cl(3)	1.713(7)
C(35)-Cl(2)	1.757(9)
C(35)-Cl(4)	1.771(9)
C(35)-H(35A)	1.0000
C(36)-Cl(6)	1.738(6)
C(36)-Cl(7)	1.764(6)
C(36)-Cl(5)	1.772(6)
C(36)-H(36A)	1.0000

C(27)-Ir(1)-C(26)	38.96(17)
C(27)-Ir(1)-N(1)	160.22(14)
C(26)-Ir(1)-N(1)	121.64(15)
C(27)-Ir(1)-C(28)	38.41(16)
C(26)-Ir(1)-C(28)	64.23(16)
N(1)-Ir(1)-C(28)	141.79(15)
C(27)-Ir(1)-C(29)	64.84(16)
C(26)-Ir(1)-C(29)	64.81(17)
N(1)-Ir(1)-C(29)	106.32(15)
C(28)-Ir(1)-C(29)	38.08(16)

C(27)-Ir(1)-C(25)	64.76(16)
C(26)-Ir(1)-C(25)	38.31(16)
N(1)-Ir(1)-C(25)	96.97(15)
C(28)-Ir(1)-C(25)	64.03(16)
C(29)-Ir(1)-C(25)	38.92(16)
C(27)-Ir(1)-N(2)	108.55(14)
C(26)-Ir(1)-N(2)	106.92(15)
N(1)-Ir(1)-N(2)	78.27(13)
C(28)-Ir(1)-N(2)	139.07(15)
C(29)-Ir(1)-N(2)	171.71(16)
C(25)-Ir(1)-N(2)	134.63(14)
C(27)-Ir(1)-Cl(1)	106.53(12)
C(26)-Ir(1)-Cl(1)	145.44(12)
N(1)-Ir(1)-Cl(1)	92.92(9)
C(28)-Ir(1)-Cl(1)	88.80(12)
C(29)-Ir(1)-Cl(1)	107.52(13)
C(25)-Ir(1)-Cl(1)	146.43(11)
N(2)-Ir(1)-Cl(1)	78.79(10)
C(1)-N(1)-C(7)	116.5(3)
C(1)-N(1)-Ir(1)	110.0(2)
C(7)-N(1)-Ir(1)	115.7(2)
C(1)-N(1)-H(1N)	106(2)
C(7)-N(1)-H(1N)	104(2)
Ir(1)-N(1)-H(1N)	103(2)
N(1)-C(1)-C(6)	113.5(3)
N(1)-C(1)-C(2)	105.8(3)
C(6)-C(1)-C(2)	109.4(4)
N(1)-C(1)-H(1A)	109.3
C(6)-C(1)-H(1A)	109.3
C(2)-C(1)-H(1A)	109.3
N(2)-C(2)-C(3)	112.9(3)
N(2)-C(2)-C(1)	109.1(3)
C(3)-C(2)-C(1)	109.0(4)
N(2)-C(2)-H(2A)	108.6
C(3)-C(2)-H(2A)	108.6
C(1)-C(2)-H(2A)	108.6
C(2)-N(2)-C(15)	114.4(3)
C(2)-N(2)-Ir(1)	111.5(3)
C(15)-N(2)-Ir(1)	118.7(3)
C(2)-N(2)-H(2N)	108(3)
C(15)-N(2)-H(2N)	108(3)
Ir(1)-N(2)-H(2N)	95(3)
C(2)-C(3)-C(4)	111.7(4)
C(2)-C(3)-H(3A)	109.3
C(4)-C(3)-H(3A)	109.3
C(2)-C(3)-H(3B)	109.3
C(4)-C(3)-H(3B)	109.3
H(3A)-C(3)-H(3B)	108.0
C(23)-C(4)-C(3)	111.0(4)
C(23)-C(4)-C(5)	112.5(4)
C(3)-C(4)-C(5)	110.4(4)
C(23)-C(4)-H(4A)	107.6
C(3)-C(4)-H(4A)	107.6
C(5)-C(4)-H(4A)	107.6
C(24)-C(5)-C(6)	111.7(4)
C(24)-C(5)-C(4)	113.2(4)
C(6)-C(5)-C(4)	110.7(4)
C(24)-C(5)-H(5A)	106.9
C(6)-C(5)-H(5A)	106.9
C(4)-C(5)-H(5A)	106.9

C(1)-C(6)-C(5)	112.6(4)
C(1)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6A)	109.1
C(1)-C(6)-H(6B)	109.1
C(5)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.8
N(1)-C(7)-C(8)	112.5(3)
N(1)-C(7)-C(14)	111.7(4)
C(8)-C(7)-C(14)	114.6(4)
N(1)-C(7)-H(7A)	105.7
C(8)-C(7)-H(7A)	105.7
C(14)-C(7)-H(7A)	105.7
C(9)-C(8)-C(13)	117.3(4)
C(9)-C(8)-C(7)	121.8(4)
C(13)-C(8)-C(7)	120.8(4)
C(10)-C(9)-C(8)	121.6(5)
C(10)-C(9)-H(9A)	119.2
C(8)-C(9)-H(9A)	119.2
C(9)-C(10)-C(11)	120.4(5)
C(9)-C(10)-H(10A)	119.8
C(11)-C(10)-H(10A)	119.8
C(12)-C(11)-C(10)	119.6(5)
C(12)-C(11)-H(11A)	120.2
C(10)-C(11)-H(11A)	120.2
C(11)-C(12)-C(13)	120.1(5)
C(11)-C(12)-H(12A)	119.9
C(13)-C(12)-H(12A)	119.9
C(12)-C(13)-C(8)	120.9(5)
C(12)-C(13)-H(13A)	119.5
C(8)-C(13)-H(13A)	119.5
C(7)-C(14)-H(14A)	109.5
C(7)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(7)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(22)-C(15)-C(16)	115.1(4)
C(22)-C(15)-N(2)	111.7(4)
C(16)-C(15)-N(2)	110.5(3)
C(22)-C(15)-H(15A)	106.3
C(16)-C(15)-H(15A)	106.3
N(2)-C(15)-H(15A)	106.3
C(21)-C(16)-C(17)	118.7(4)
C(21)-C(16)-C(15)	119.5(4)
C(17)-C(16)-C(15)	121.8(4)
C(18)-C(17)-C(16)	120.4(5)
C(18)-C(17)-H(17A)	119.8
C(16)-C(17)-H(17A)	119.8
C(19)-C(18)-C(17)	120.3(5)
C(19)-C(18)-H(18A)	119.8
C(17)-C(18)-H(18A)	119.8
C(18)-C(19)-C(20)	120.1(4)
C(18)-C(19)-H(19A)	120.0
C(20)-C(19)-H(19A)	120.0
C(21)-C(20)-C(19)	119.9(5)
C(21)-C(20)-H(20A)	120.1
C(19)-C(20)-H(20A)	120.1
C(20)-C(21)-C(16)	120.6(5)
C(20)-C(21)-H(21A)	119.7
C(16)-C(21)-H(21A)	119.7

C(15)-C(22)-H(22A)	109.5
C(15)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(15)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(4)-C(23)-H(23A)	109.5
C(4)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(4)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(5)-C(24)-H(24A)	109.5
C(5)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(5)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(29)	108.1(4)
C(26)-C(25)-C(30)	126.5(4)
C(29)-C(25)-C(30)	125.2(4)
C(26)-C(25)-Ir(1)	70.6(2)
C(29)-C(25)-Ir(1)	70.4(2)
C(30)-C(25)-Ir(1)	129.0(3)
C(25)-C(26)-C(27)	107.9(4)
C(25)-C(26)-C(31)	125.1(4)
C(27)-C(26)-C(31)	126.5(4)
C(25)-C(26)-Ir(1)	71.1(2)
C(27)-C(26)-Ir(1)	69.9(2)
C(31)-C(26)-Ir(1)	130.9(3)
C(28)-C(27)-C(26)	107.4(4)
C(28)-C(27)-C(32)	124.7(4)
C(26)-C(27)-C(32)	127.2(4)
C(28)-C(27)-Ir(1)	71.6(2)
C(26)-C(27)-Ir(1)	71.2(2)
C(32)-C(27)-Ir(1)	130.1(3)
C(29)-C(28)-C(27)	109.5(4)
C(29)-C(28)-C(33)	124.9(4)
C(27)-C(28)-C(33)	125.6(4)
C(29)-C(28)-Ir(1)	71.0(2)
C(27)-C(28)-Ir(1)	70.0(2)
C(33)-C(28)-Ir(1)	127.2(3)
C(28)-C(29)-C(25)	107.1(4)
C(28)-C(29)-C(34)	125.6(4)
C(25)-C(29)-C(34)	126.8(4)
C(28)-C(29)-Ir(1)	70.9(2)
C(25)-C(29)-Ir(1)	70.7(2)
C(34)-C(29)-Ir(1)	130.0(3)
C(25)-C(30)-H(30A)	109.5
C(25)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(25)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5

C(27)-C(32)-H(32A)	109.5
C(27)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(27)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(28)-C(33)-H(33A)	109.5
C(28)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(28)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(29)-C(34)-H(34A)	109.5
C(29)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(29)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
F(4)-B(1)-F(2)	110.9(5)
F(4)-B(1)-F(1)	109.1(5)
F(2)-B(1)-F(1)	110.4(4)
F(4)-B(1)-F(3)	108.4(4)
F(2)-B(1)-F(3)	109.1(4)
F(1)-B(1)-F(3)	108.9(4)
Cl(3)-C(35)-Cl(2)	110.4(5)
Cl(3)-C(35)-Cl(4)	111.6(5)
Cl(2)-C(35)-Cl(4)	109.9(4)
Cl(3)-C(35)-H(35A)	108.2
Cl(2)-C(35)-H(35A)	108.2
Cl(4)-C(35)-H(35A)	108.2
Cl(6)-C(36)-Cl(7)	109.5(3)
Cl(6)-C(36)-Cl(5)	111.6(3)
Cl(7)-C(36)-Cl(5)	110.8(3)
Cl(6)-C(36)-H(36A)	108.3
Cl(7)-C(36)-H(36A)	108.3
Cl(5)-C(36)-H(36A)	108.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mfmc1. 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)	15(1)	13(1)	-2(1)	0(1)	-2(1)
Cl(1)	22(1)	27(1)	18(1)	0(1)	4(1)	-7(1)
N(1)	15(2)	12(2)	16(2)	0(2)	0(1)	-2(2)
C(1)	23(2)	13(2)	14(2)	1(2)	-1(2)	-1(2)
C(2)	21(2)	21(2)	7(2)	2(2)	-2(2)	4(2)
N(2)	27(2)	15(2)	15(2)	-1(2)	-4(2)	0(2)
C(3)	30(3)	11(2)	22(2)	-4(2)	-3(2)	0(2)
C(4)	41(3)	12(2)	20(2)	-3(2)	-5(2)	-4(2)
C(5)	37(3)	19(2)	21(3)	-6(2)	-5(2)	-8(2)
C(6)	28(3)	18(2)	17(3)	4(2)	-5(2)	-5(2)
C(7)	21(2)	19(2)	18(3)	-1(2)	-4(2)	4(2)
C(8)	27(3)	8(2)	23(3)	-2(2)	-6(2)	1(2)
C(9)	19(2)	14(2)	34(3)	3(2)	-4(2)	0(2)
C(10)	40(3)	20(2)	24(3)	6(2)	2(2)	-6(2)
C(11)	51(4)	21(3)	23(3)	5(2)	-10(3)	-6(2)
C(12)	33(3)	24(3)	33(3)	1(2)	-17(3)	3(2)
C(13)	29(3)	22(2)	26(3)	-1(2)	-4(2)	2(2)
C(14)	21(3)	48(3)	26(3)	4(3)	5(2)	7(2)
C(15)	20(2)	20(2)	14(2)	-3(2)	-2(2)	7(2)
C(16)	23(2)	17(2)	16(2)	4(2)	-10(2)	-1(2)
C(17)	26(3)	16(2)	26(3)	1(2)	-5(2)	-1(2)
C(18)	33(3)	28(3)	25(3)	-5(3)	-9(3)	0(2)
C(19)	47(3)	22(3)	28(3)	4(2)	-15(3)	-1(3)
C(20)	38(3)	36(3)	16(3)	6(2)	-4(2)	-4(2)
C(21)	35(3)	24(3)	20(3)	2(2)	-6(2)	0(2)
C(22)	23(3)	22(2)	22(3)	0(2)	-2(2)	1(2)
C(23)	54(4)	41(3)	21(3)	-8(3)	-4(2)	2(3)
C(24)	35(3)	34(3)	32(3)	0(3)	-8(2)	-13(3)
C(25)	24(3)	15(2)	17(2)	-9(2)	1(2)	-8(2)
C(26)	17(2)	16(2)	23(3)	-9(2)	3(2)	-5(2)
C(27)	17(2)	20(2)	20(2)	-6(2)	-6(2)	0(2)
C(28)	22(3)	20(2)	15(2)	-9(2)	-3(2)	-3(2)
C(29)	22(2)	18(2)	18(2)	-8(2)	-5(2)	1(2)
C(30)	34(3)	22(2)	24(3)	3(2)	1(2)	-10(2)
C(31)	17(2)	24(2)	31(3)	-8(2)	5(2)	-6(2)
C(32)	23(2)	28(3)	23(3)	-2(2)	-4(2)	4(2)
C(33)	28(3)	33(3)	19(3)	-6(2)	5(2)	3(2)
C(34)	26(3)	26(3)	26(3)	-8(2)	-1(2)	6(2)
B(1)	30(3)	36(4)	21(3)	4(3)	5(3)	4(3)
F(1)	43(2)	46(2)	45(2)	-9(2)	4(2)	16(2)
F(2)	59(2)	95(3)	26(2)	20(2)	-5(2)	9(2)
F(3)	26(2)	40(2)	26(1)	11(1)	9(1)	5(1)
F(4)	43(2)	44(2)	78(3)	12(2)	7(2)	-20(2)
C(35)	129(7)	58(5)	43(4)	-6(4)	-10(5)	10(5)
Cl(2)	136(2)	176(3)	68(2)	-3(2)	-10(2)	82(2)
Cl(3)	88(1)	70(1)	73(1)	1(1)	-24(1)	-10(1)
Cl(4)	127(2)	81(1)	85(2)	-17(1)	13(2)	-29(2)
C(36)	36(3)	42(3)	45(3)	6(3)	6(2)	-3(3)
Cl(5)	67(1)	47(1)	55(1)	-5(1)	14(1)	-2(1)
Cl(6)	50(1)	48(1)	44(1)	10(1)	-9(1)	-6(1)
Cl(7)	49(1)	40(1)	51(1)	4(1)	4(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mfmc1.

	x	y	z	U(eq)
H(1N)	3200(20)	6300(20)	2107(16)	14(11)
H(1A)	4485	7495	1656	20
H(2A)	2494	7558	2216	20
H(2N)	3120(30)	7880(30)	780(20)	43(15)
H(3A)	2600	8901	1960	25
H(3B)	3726	8794	1714	25
H(4A)	3732	9259	2896	29
H(5A)	4570	8221	3527	31
H(6A)	4916	7080	2839	25
H(6B)	3790	7145	3094	25
H(7A)	4284	5403	1623	23
H(9A)	3238	5546	2944	27
H(10A)	3484	5250	4151	34
H(11A)	5081	5117	4611	38
H(12A)	6428	5294	3849	36
H(13A)	6189	5672	2645	31
H(14A)	5974	5717	1538	48
H(14B)	5706	6607	1655	48
H(14C)	5323	6164	947	48
H(15A)	1348	7676	538	22
H(17A)	768	9315	1394	27
H(18A)	920	10563	944	34
H(19A)	1994	10822	-11	39
H(20A)	2850	9816	-574	36
H(21A)	2687	8559	-140	32
H(22A)	904	7322	1724	33
H(22B)	262	8039	1450	33
H(22C)	1156	8172	2005	33
H(23A)	2131	8859	3240	58
H(23B)	2917	8651	3859	58
H(23C)	2516	7992	3326	58
H(24A)	5948	8203	2774	50
H(24B)	5507	9055	2840	50
H(24C)	5307	8555	2124	50
H(30A)	1879	4350	1386	40
H(30B)	1682	5111	1855	40
H(30C)	2784	4796	1753	40
H(31A)	88	5641	757	36
H(31B)	313	6546	732	36
H(31C)	607	6053	1434	36
H(32A)	1123	6363	-1051	38
H(32B)	1832	7066	-840	38
H(32C)	824	6933	-405	38
H(33A)	3149	5487	-1308	40
H(33B)	4101	5711	-839	40
H(33C)	3371	6371	-1122	40
H(34A)	3764	4302	5	39
H(34B)	3944	4503	842	39
H(34C)	4500	4984	224	39
H(35A)	5229	7585	5770	92
H(36A)	9222	6518	2571	49

Table 6. Torsion angles [°] for mfmc1.

C(27)-Ir(1)-N(1)-C(1)	-136.4(4)
C(26)-Ir(1)-N(1)-C(1)	-126.6(3)
C(28)-Ir(1)-N(1)-C(1)	145.8(3)
C(29)-Ir(1)-N(1)-C(1)	163.3(3)
C(25)-Ir(1)-N(1)-C(1)	-158.1(3)
N(2)-Ir(1)-N(1)-C(1)	-23.8(3)
Cl(1)-Ir(1)-N(1)-C(1)	54.1(3)
C(27)-Ir(1)-N(1)-C(7)	89.0(5)
C(26)-Ir(1)-N(1)-C(7)	98.8(3)
C(28)-Ir(1)-N(1)-C(7)	11.2(4)
C(29)-Ir(1)-N(1)-C(7)	28.7(3)
C(25)-Ir(1)-N(1)-C(7)	67.3(3)
N(2)-Ir(1)-N(1)-C(7)	-158.5(3)
Cl(1)-Ir(1)-N(1)-C(7)	-80.5(3)
C(7)-N(1)-C(1)-C(6)	-57.3(5)
Ir(1)-N(1)-C(1)-C(6)	168.6(3)
C(7)-N(1)-C(1)-C(2)	-177.2(3)
Ir(1)-N(1)-C(1)-C(2)	48.6(3)
N(1)-C(1)-C(2)-N(2)	-54.0(4)
C(6)-C(1)-C(2)-N(2)	-176.6(3)
N(1)-C(1)-C(2)-C(3)	-177.6(3)
C(6)-C(1)-C(2)-C(3)	59.8(4)
C(3)-C(2)-N(2)-C(15)	-66.3(5)
C(1)-C(2)-N(2)-C(15)	172.4(3)
C(3)-C(2)-N(2)-Ir(1)	155.6(3)
C(1)-C(2)-N(2)-Ir(1)	34.3(4)
C(27)-Ir(1)-N(2)-C(2)	154.8(3)
C(26)-Ir(1)-N(2)-C(2)	113.8(3)
N(1)-Ir(1)-N(2)-C(2)	-5.9(3)
C(28)-Ir(1)-N(2)-C(2)	-176.2(3)
C(29)-Ir(1)-N(2)-C(2)	118.5(10)
C(25)-Ir(1)-N(2)-C(2)	82.3(4)
Cl(1)-Ir(1)-N(2)-C(2)	-101.3(3)
C(27)-Ir(1)-N(2)-C(15)	18.7(3)
C(26)-Ir(1)-N(2)-C(15)	-22.3(3)
N(1)-Ir(1)-N(2)-C(15)	-142.1(3)
C(28)-Ir(1)-N(2)-C(15)	47.7(4)
C(29)-Ir(1)-N(2)-C(15)	-17.6(12)
C(25)-Ir(1)-N(2)-C(15)	-53.8(4)
Cl(1)-Ir(1)-N(2)-C(15)	122.5(3)
N(2)-C(2)-C(3)-C(4)	178.3(4)
C(1)-C(2)-C(3)-C(4)	-60.4(5)
C(2)-C(3)-C(4)-C(23)	-68.6(5)
C(2)-C(3)-C(4)-C(5)	56.9(5)
C(23)-C(4)-C(5)-C(24)	-161.5(4)
C(3)-C(4)-C(5)-C(24)	73.9(5)
C(23)-C(4)-C(5)-C(6)	72.2(5)
C(3)-C(4)-C(5)-C(6)	-52.4(5)
N(1)-C(1)-C(6)-C(5)	-175.8(4)
C(2)-C(1)-C(6)-C(5)	-57.9(5)
C(24)-C(5)-C(6)-C(1)	-72.9(5)
C(4)-C(5)-C(6)-C(1)	54.3(5)
C(1)-N(1)-C(7)-C(8)	75.0(5)
Ir(1)-N(1)-C(7)-C(8)	-153.4(3)
C(1)-N(1)-C(7)-C(14)	-55.5(5)
Ir(1)-N(1)-C(7)-C(14)	76.1(4)
N(1)-C(7)-C(8)-C(9)	44.0(6)
C(14)-C(7)-C(8)-C(9)	173.0(4)

N(1)-C(7)-C(8)-C(13)	-137.5(4)
C(14)-C(7)-C(8)-C(13)	-8.5(6)
C(13)-C(8)-C(9)-C(10)	2.4(7)
C(7)-C(8)-C(9)-C(10)	-179.1(4)
C(8)-C(9)-C(10)-C(11)	-2.5(7)
C(9)-C(10)-C(11)-C(12)	0.2(7)
C(10)-C(11)-C(12)-C(13)	2.0(7)
C(11)-C(12)-C(13)-C(8)	-2.0(7)
C(9)-C(8)-C(13)-C(12)	-0.2(7)
C(7)-C(8)-C(13)-C(12)	-178.7(4)
C(2)-N(2)-C(15)-C(22)	-39.6(5)
Ir(1)-N(2)-C(15)-C(22)	95.4(4)
C(2)-N(2)-C(15)-C(16)	89.9(4)
Ir(1)-N(2)-C(15)-C(16)	-135.2(3)
C(22)-C(15)-C(16)-C(21)	-178.3(4)
N(2)-C(15)-C(16)-C(21)	54.1(5)
C(22)-C(15)-C(16)-C(17)	-1.0(6)
N(2)-C(15)-C(16)-C(17)	-128.6(4)
C(21)-C(16)-C(17)-C(18)	-1.5(7)
C(15)-C(16)-C(17)-C(18)	-178.8(4)
C(16)-C(17)-C(18)-C(19)	-0.6(7)
C(17)-C(18)-C(19)-C(20)	2.2(7)
C(18)-C(19)-C(20)-C(21)	-1.7(7)
C(19)-C(20)-C(21)-C(16)	-0.4(7)
C(17)-C(16)-C(21)-C(20)	1.9(7)
C(15)-C(16)-C(21)-C(20)	179.3(4)
C(27)-Ir(1)-C(25)-C(26)	-37.8(2)
N(1)-Ir(1)-C(25)-C(26)	134.2(2)
C(28)-Ir(1)-C(25)-C(26)	-80.6(3)
C(29)-Ir(1)-C(25)-C(26)	-118.4(4)
N(2)-Ir(1)-C(25)-C(26)	53.9(3)
Cl(1)-Ir(1)-C(25)-C(26)	-119.7(3)
C(27)-Ir(1)-C(25)-C(29)	80.6(3)
C(26)-Ir(1)-C(25)-C(29)	118.4(4)
N(1)-Ir(1)-C(25)-C(29)	-107.4(2)
C(28)-Ir(1)-C(25)-C(29)	37.8(2)
N(2)-Ir(1)-C(25)-C(29)	172.2(2)
Cl(1)-Ir(1)-C(25)-C(29)	-1.3(4)
C(27)-Ir(1)-C(25)-C(30)	-159.5(5)
C(26)-Ir(1)-C(25)-C(30)	-121.7(5)
N(1)-Ir(1)-C(25)-C(30)	12.5(4)
C(28)-Ir(1)-C(25)-C(30)	157.7(5)
C(29)-Ir(1)-C(25)-C(30)	119.9(5)
N(2)-Ir(1)-C(25)-C(30)	-67.9(5)
Cl(1)-Ir(1)-C(25)-C(30)	118.6(4)
C(29)-C(25)-C(26)-C(27)	-0.3(4)
C(30)-C(25)-C(26)-C(27)	-174.8(4)
Ir(1)-C(25)-C(26)-C(27)	60.5(3)
C(29)-C(25)-C(26)-C(31)	172.0(4)
C(30)-C(25)-C(26)-C(31)	-2.5(7)
Ir(1)-C(25)-C(26)-C(31)	-127.3(4)
C(29)-C(25)-C(26)-Ir(1)	-60.7(3)
C(30)-C(25)-C(26)-Ir(1)	124.8(4)
C(27)-Ir(1)-C(26)-C(25)	118.1(3)
N(1)-Ir(1)-C(26)-C(25)	-56.6(3)
C(28)-Ir(1)-C(26)-C(25)	80.0(3)
C(29)-Ir(1)-C(26)-C(25)	37.7(2)
N(2)-Ir(1)-C(26)-C(25)	-143.1(2)
Cl(1)-Ir(1)-C(26)-C(25)	122.1(2)
N(1)-Ir(1)-C(26)-C(27)	-174.8(2)

C(28)-Ir(1)-C(26)-C(27)	-38.1(2)
C(29)-Ir(1)-C(26)-C(27)	-80.5(3)
C(25)-Ir(1)-C(26)-C(27)	-118.1(3)
N(2)-Ir(1)-C(26)-C(27)	98.8(2)
Cl(1)-Ir(1)-C(26)-C(27)	4.0(4)
C(27)-Ir(1)-C(26)-C(31)	-121.4(5)
N(1)-Ir(1)-C(26)-C(31)	63.9(5)
C(28)-Ir(1)-C(26)-C(31)	-159.5(5)
C(29)-Ir(1)-C(26)-C(31)	158.2(5)
C(25)-Ir(1)-C(26)-C(31)	120.5(5)
N(2)-Ir(1)-C(26)-C(31)	-22.6(5)
Cl(1)-Ir(1)-C(26)-C(31)	-117.4(4)
C(25)-C(26)-C(27)-C(28)	1.6(4)
C(31)-C(26)-C(27)-C(28)	-170.5(4)
Ir(1)-C(26)-C(27)-C(28)	62.8(3)
C(25)-C(26)-C(27)-C(32)	172.2(4)
C(31)-C(26)-C(27)-C(32)	0.1(7)
Ir(1)-C(26)-C(27)-C(32)	-126.6(4)
C(25)-C(26)-C(27)-Ir(1)	-61.2(3)
C(31)-C(26)-C(27)-Ir(1)	126.6(4)
C(26)-Ir(1)-C(27)-C(28)	-116.5(3)
N(1)-Ir(1)-C(27)-C(28)	-103.3(5)
C(29)-Ir(1)-C(27)-C(28)	-36.2(3)
C(25)-Ir(1)-C(27)-C(28)	-79.4(3)
N(2)-Ir(1)-C(27)-C(28)	149.3(2)
Cl(1)-Ir(1)-C(27)-C(28)	65.8(2)
N(1)-Ir(1)-C(27)-C(26)	13.2(6)
C(28)-Ir(1)-C(27)-C(26)	116.5(3)
C(29)-Ir(1)-C(27)-C(26)	80.4(3)
C(25)-Ir(1)-C(27)-C(26)	37.2(2)
N(2)-Ir(1)-C(27)-C(26)	-94.2(2)
Cl(1)-Ir(1)-C(27)-C(26)	-177.6(2)
C(26)-Ir(1)-C(27)-C(32)	123.3(5)
N(1)-Ir(1)-C(27)-C(32)	136.5(4)
C(28)-Ir(1)-C(27)-C(32)	-120.2(5)
C(29)-Ir(1)-C(27)-C(32)	-156.4(5)
C(25)-Ir(1)-C(27)-C(32)	160.4(5)
N(2)-Ir(1)-C(27)-C(32)	29.1(4)
Cl(1)-Ir(1)-C(27)-C(32)	-54.4(4)
C(26)-C(27)-C(28)-C(29)	-2.3(5)
C(32)-C(27)-C(28)-C(29)	-173.2(4)
Ir(1)-C(27)-C(28)-C(29)	60.2(3)
C(26)-C(27)-C(28)-C(33)	175.4(4)
C(32)-C(27)-C(28)-C(33)	4.4(7)
Ir(1)-C(27)-C(28)-C(33)	-122.1(4)
C(26)-C(27)-C(28)-Ir(1)	-62.6(3)
C(32)-C(27)-C(28)-Ir(1)	126.5(4)
C(27)-Ir(1)-C(28)-C(29)	-120.0(4)
C(26)-Ir(1)-C(28)-C(29)	-81.4(3)
N(1)-Ir(1)-C(28)-C(29)	27.8(4)
C(25)-Ir(1)-C(28)-C(29)	-38.6(3)
N(2)-Ir(1)-C(28)-C(29)	-167.7(3)
Cl(1)-Ir(1)-C(28)-C(29)	121.0(3)
C(26)-Ir(1)-C(28)-C(27)	38.7(3)
N(1)-Ir(1)-C(28)-C(27)	147.8(2)
C(29)-Ir(1)-C(28)-C(27)	120.0(4)
C(25)-Ir(1)-C(28)-C(27)	81.4(3)
N(2)-Ir(1)-C(28)-C(27)	-47.7(4)
Cl(1)-Ir(1)-C(28)-C(27)	-119.0(2)
C(27)-Ir(1)-C(28)-C(33)	120.1(5)

C(26)-Ir(1)-C(28)-C(33)	158.7(4)
N(1)-Ir(1)-C(28)-C(33)	-92.1(4)
C(29)-Ir(1)-C(28)-C(33)	-119.9(5)
C(25)-Ir(1)-C(28)-C(33)	-158.5(4)
N(2)-Ir(1)-C(28)-C(33)	72.4(5)
Cl(1)-Ir(1)-C(28)-C(33)	1.1(4)
C(27)-C(28)-C(29)-C(25)	2.1(5)
C(33)-C(28)-C(29)-C(25)	-175.6(4)
Ir(1)-C(28)-C(29)-C(25)	61.8(3)
C(27)-C(28)-C(29)-C(34)	174.3(4)
C(33)-C(28)-C(29)-C(34)	-3.4(7)
Ir(1)-C(28)-C(29)-C(34)	-126.1(4)
C(27)-C(28)-C(29)-Ir(1)	-59.7(3)
C(33)-C(28)-C(29)-Ir(1)	122.6(4)
C(26)-C(25)-C(29)-C(28)	-1.1(5)
C(30)-C(25)-C(29)-C(28)	173.5(4)
Ir(1)-C(25)-C(29)-C(28)	-62.0(3)
C(26)-C(25)-C(29)-C(34)	-173.1(4)
C(30)-C(25)-C(29)-C(34)	1.5(7)
Ir(1)-C(25)-C(29)-C(34)	126.0(4)
C(26)-C(25)-C(29)-Ir(1)	60.8(3)
C(30)-C(25)-C(29)-Ir(1)	-124.6(4)
C(27)-Ir(1)-C(29)-C(28)	36.5(3)
C(26)-Ir(1)-C(29)-C(28)	79.7(3)
N(1)-Ir(1)-C(29)-C(28)	-162.5(2)
C(25)-Ir(1)-C(29)-C(28)	116.8(4)
N(2)-Ir(1)-C(29)-C(28)	74.8(11)
Cl(1)-Ir(1)-C(29)-C(28)	-64.0(3)
C(27)-Ir(1)-C(29)-C(25)	-80.3(3)
C(26)-Ir(1)-C(29)-C(25)	-37.1(3)
N(1)-Ir(1)-C(29)-C(25)	80.7(3)
C(28)-Ir(1)-C(29)-C(25)	-116.8(4)
N(2)-Ir(1)-C(29)-C(25)	-42.0(11)
Cl(1)-Ir(1)-C(29)-C(25)	179.2(2)
C(27)-Ir(1)-C(29)-C(34)	157.4(5)
C(26)-Ir(1)-C(29)-C(34)	-159.4(5)
N(1)-Ir(1)-C(29)-C(34)	-41.6(4)
C(28)-Ir(1)-C(29)-C(34)	120.9(5)
C(25)-Ir(1)-C(29)-C(34)	-122.3(5)
N(2)-Ir(1)-C(29)-C(34)	-164.3(9)
Cl(1)-Ir(1)-C(29)-C(34)	56.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mfmc1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...F(3)	0.978(5)	2.093(18)	3.007(4)	155(3)
N(2)-H(2N)...Cl(1)	0.978(5)	2.30(4)	2.936(4)	122(4)

Symmetry transformations used to generate equivalent atoms: