Supporting Information

Supporting Information for:

Mono and dimetallic pyrene-imidazolylidene complexes of iridium (III) for the deuteration of organic substrates and the C-C coupling of alcohols

by

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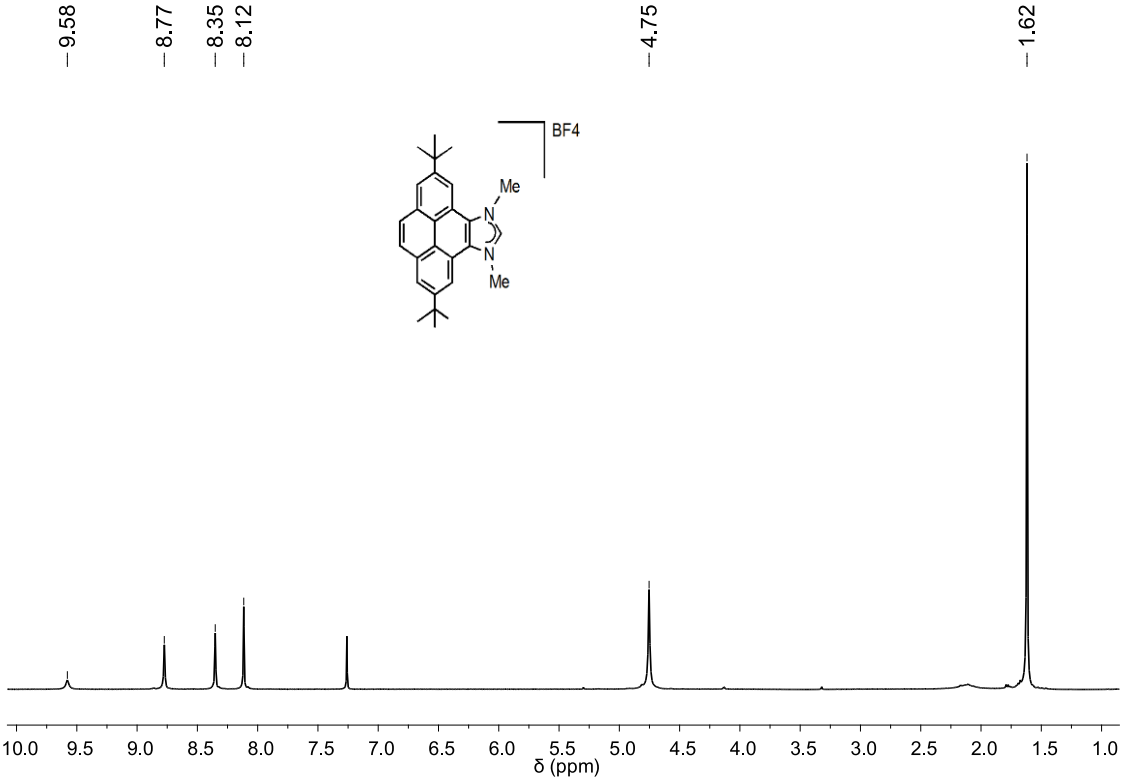
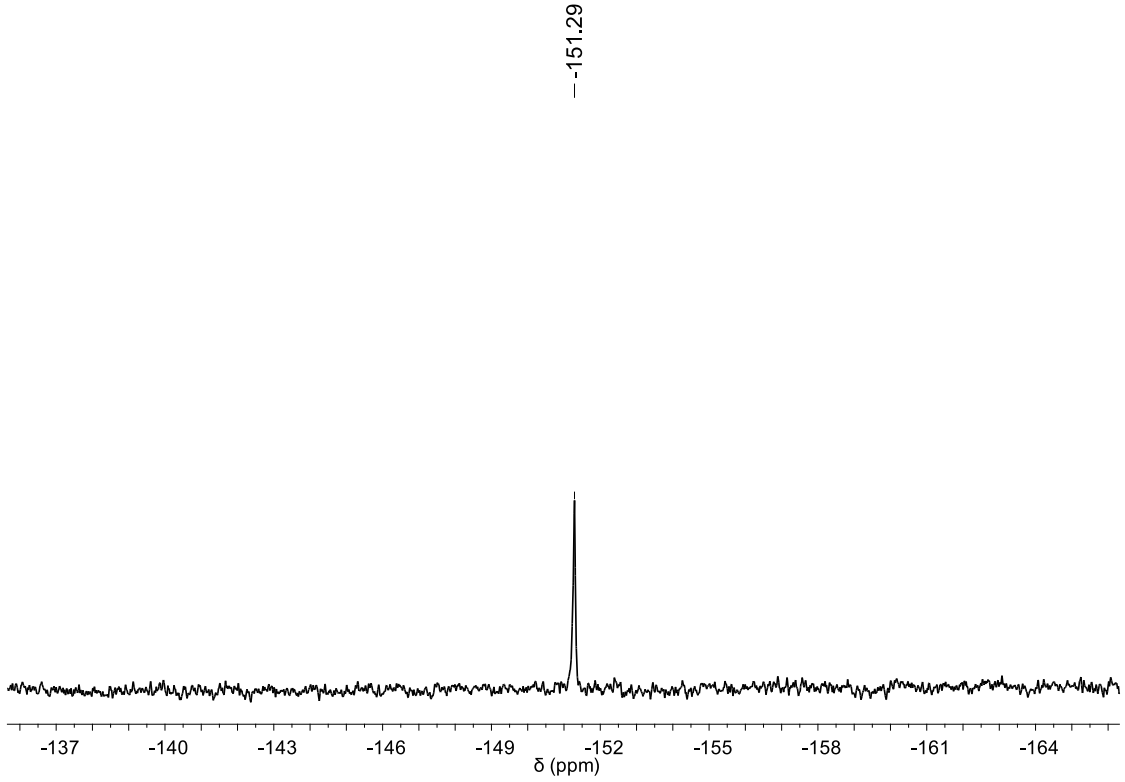
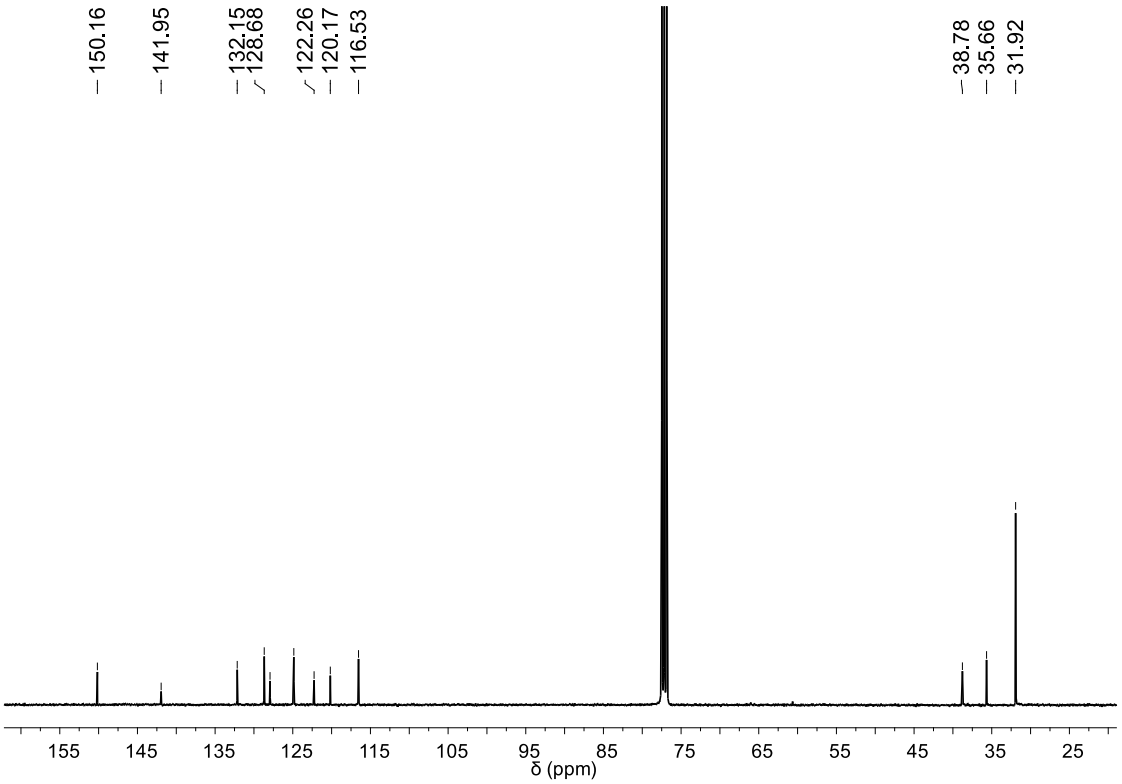
1. Spectroscopic data

1.1. ^{1}H, ^{19}F and ^{13}C NMR spectra of 2






150.16
141.95
132.15
128.68
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120.17
116.53
38.78
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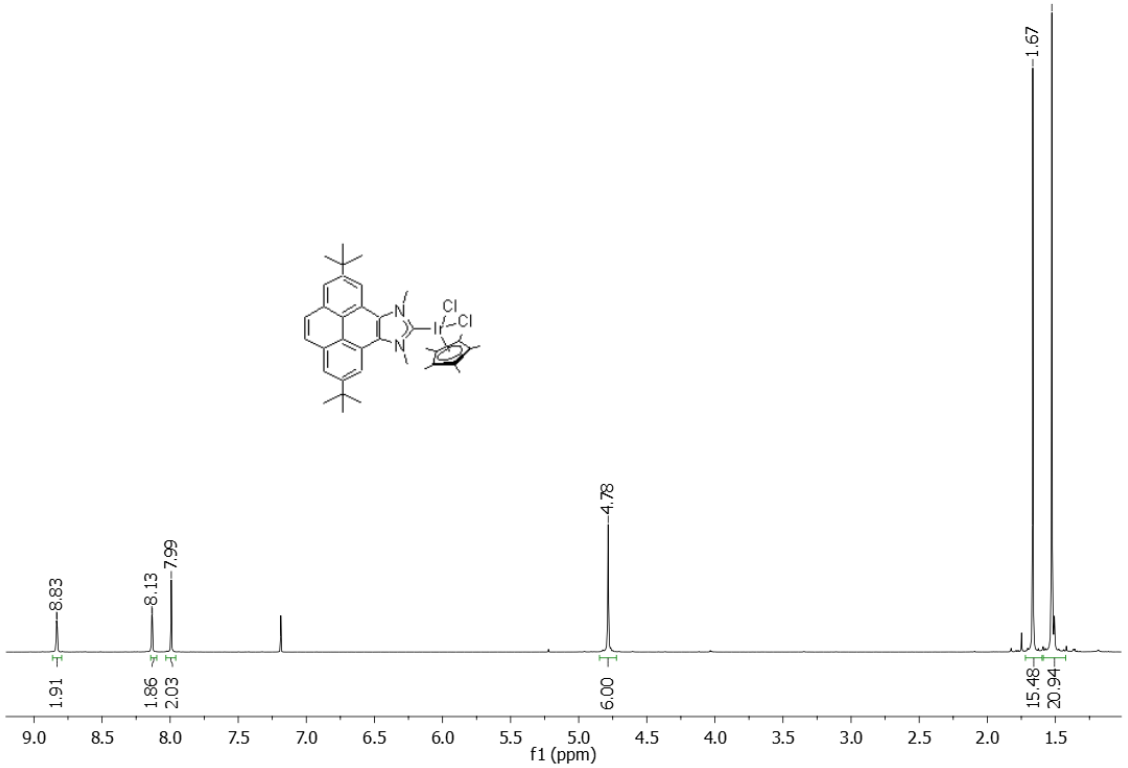
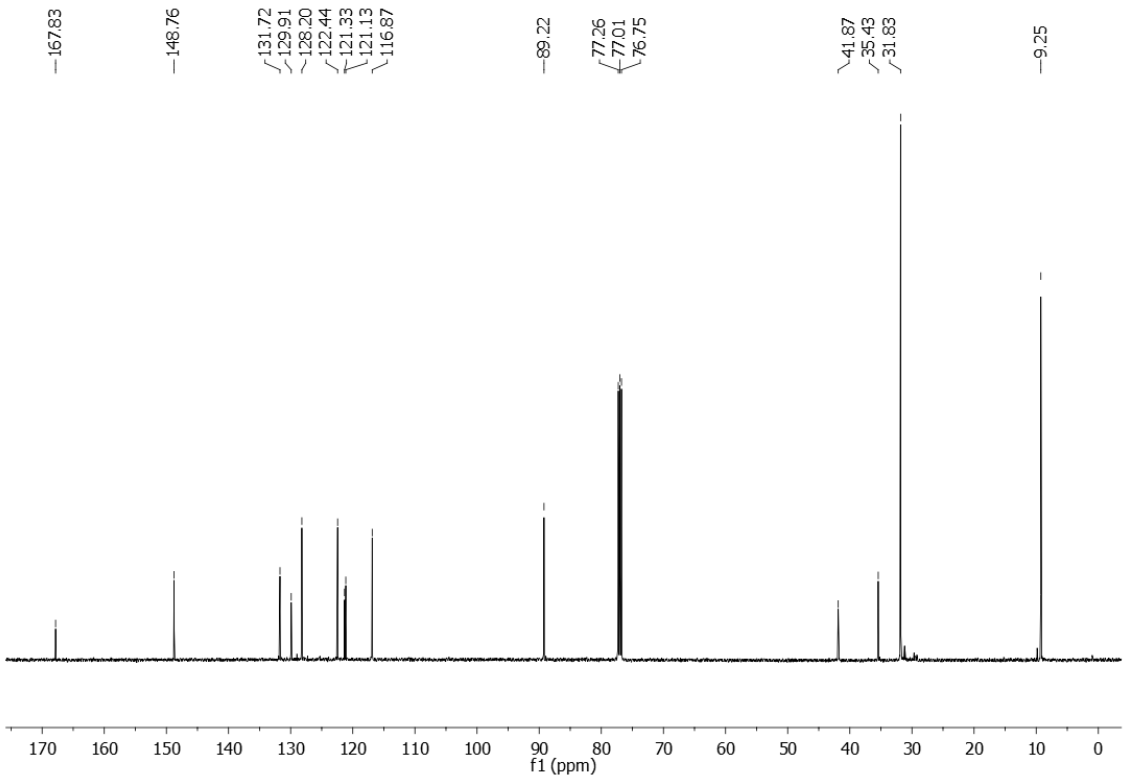
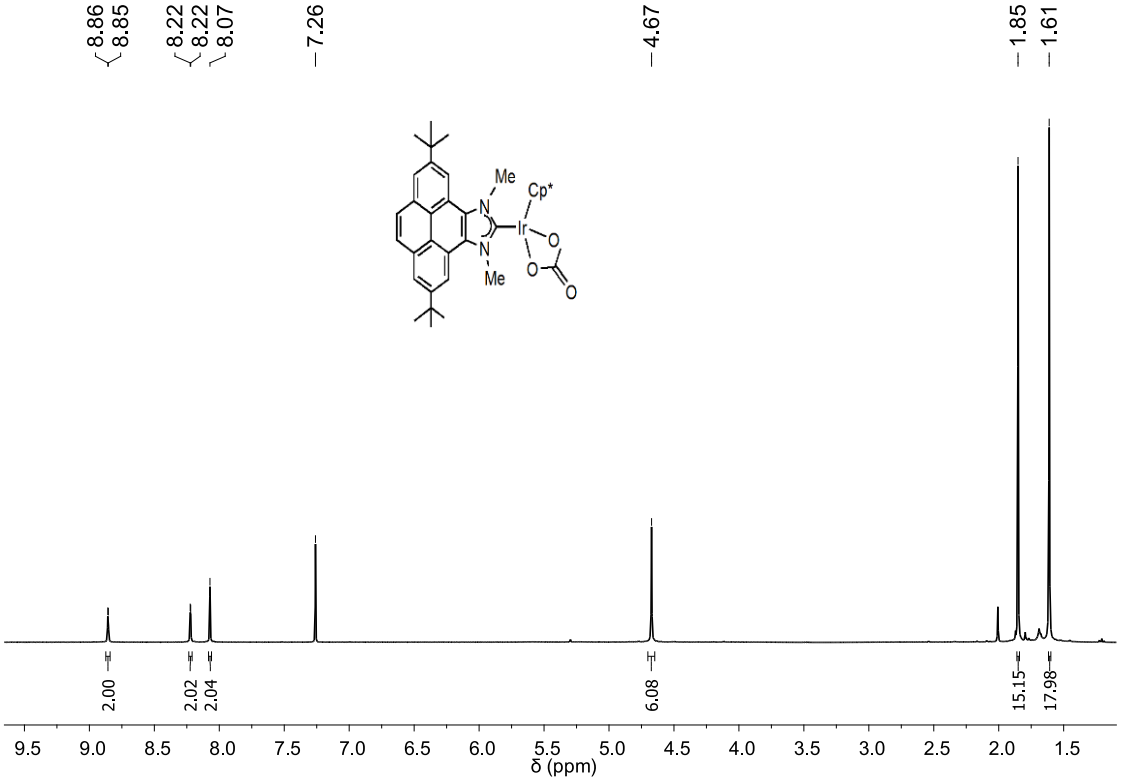
31.92
155
145
135
125
115
105
95
85
75
65
55
45
35
25
δ (ppm)

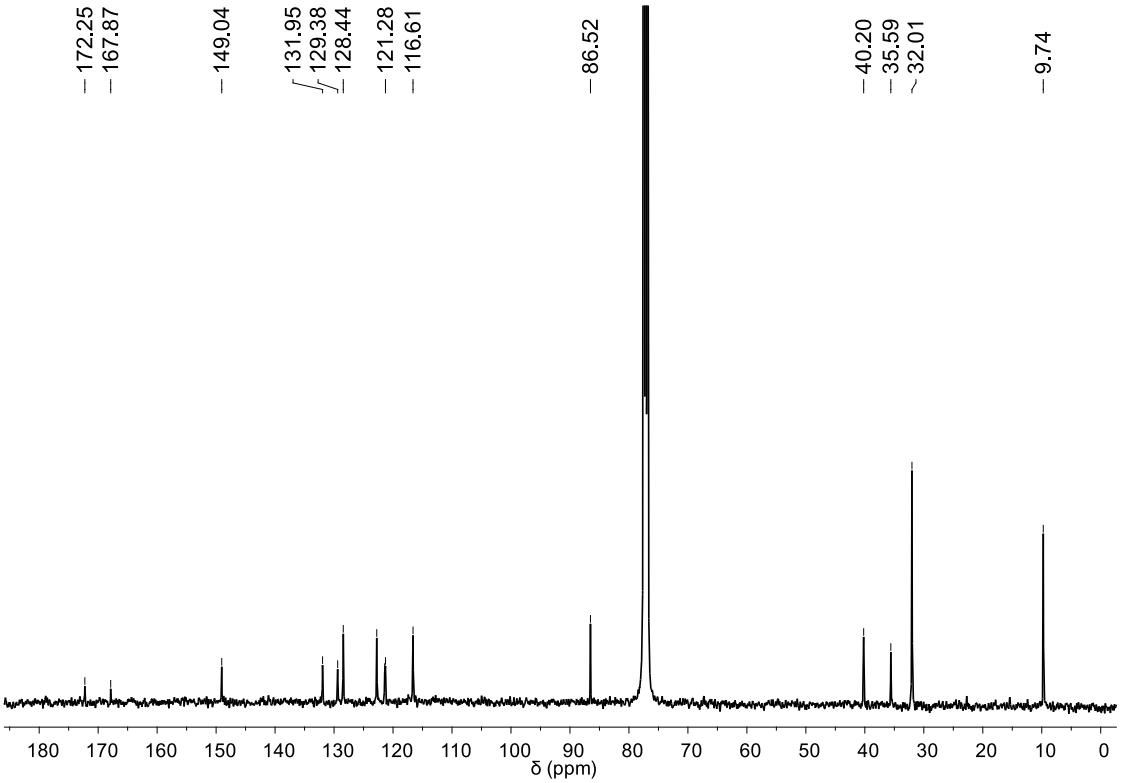
1.2. ^{1}H and ^{13}C NMR spectra of 3



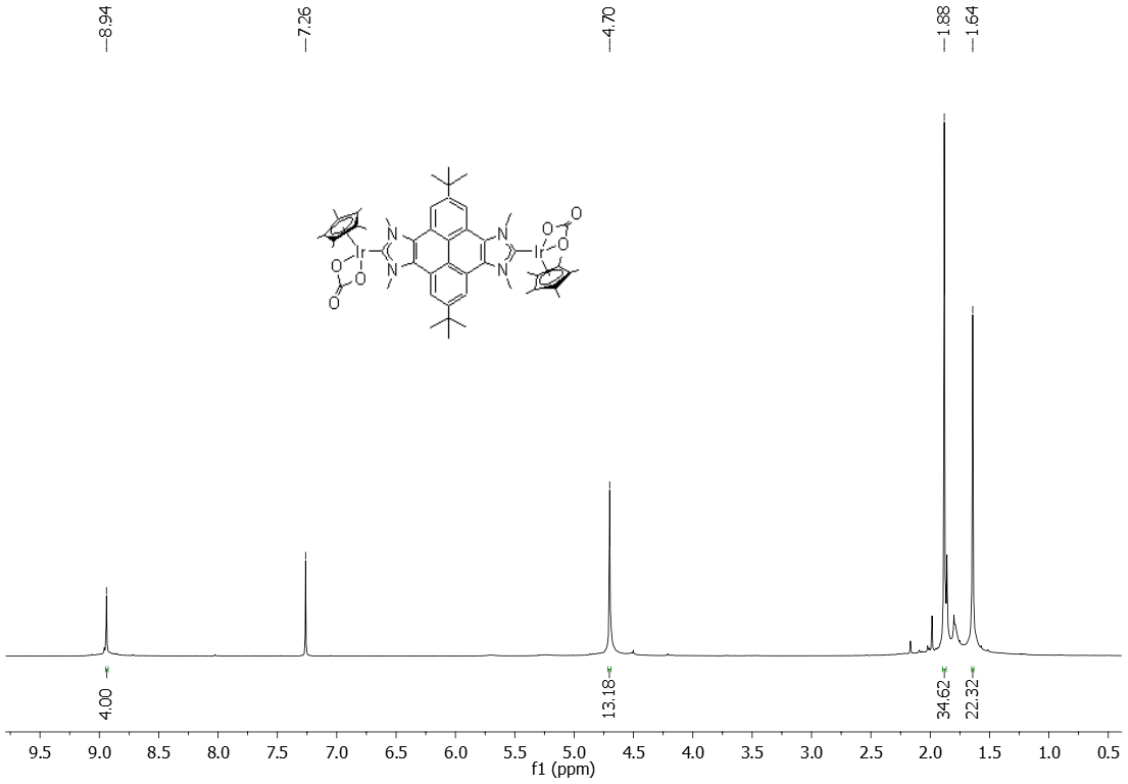


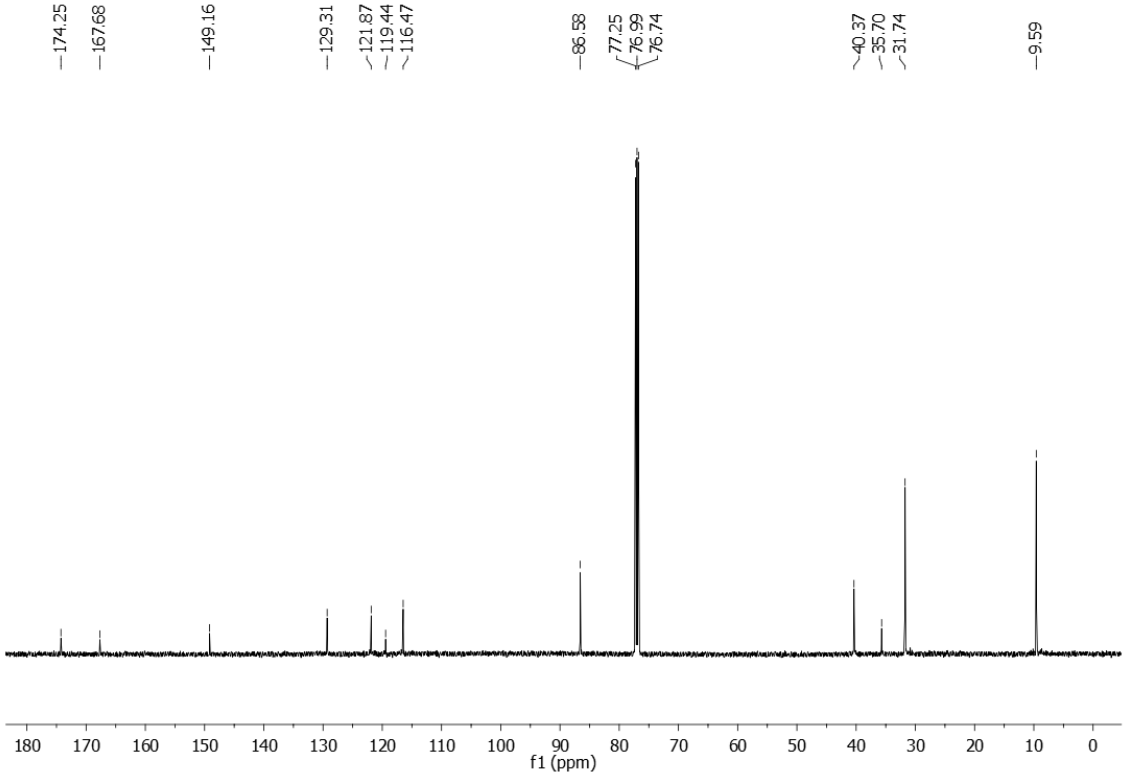
1.3. ^{1}H and ^{13}C NMR spectra of 4





1.4. ^{1}H and ^{13}C NMR spectra of 6





2. X-Ray crystallography

X-Ray diffraction studies for complexes 3, 4 and 6. Crystals suitable for X-ray study of complexes **3**, **4** and **6** were obtained by slow diffusion of hexane into a concentrated solution of the complex in chloroform. Diffraction data was collected on an Agilent SuperNova diffractometer equipped with an Atlas CCD detector using Mo-Kα radiation (λ = 0.71073 Å). Single crystals were mounted on a MicroMount® polymer tip (MiteGen) in a random orientation. Absorption corrections based on the gaussian method were applied. Using Olex2[1] the structures of all the complexes were solved using Charge Flipping[2] in Superflip and refined with ShelXL[3] refinement package using Least Squares minimisation. Key details of the crystals and structure refinement data are summarized in Supplementary Table S1. Further crystallographic details may be found in the CIF files, which were deposited at the Cambridge Crystallographic Data Centre, Cambridge, UK. The reference numbers for complexes **3**, **4** and **6** were assigned as 1495410, 1495845 and 1495411, respectively.

Table S1. Summary of crystal data, data collection, and structure refinement details

	complex **3**	complex **4**	complex **6**
Empirical formula	$C_{44}H_{45}Cl_2IrN_2$	$C_{40}H_{46}Cl_6IrN_2O_3$	$C_{29}H_{35}Cl_9IrN_2O_3$
Formula weight	864.92	1008.69	970.84
Temperature/K	200(2)	160.3(9)	200.0(4)
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/c$	Pnma	$P2_1/n$
a/Å	11.4266(3)	14.3211(6)	13.2410(5)
b/Å	21.9900(7)	24.2943(9)	21.8290(9)
c/Å	16.1613(5)	12.1511(4)	13.3907(5)
α/°	90	90	90
β/°	96.611(3)	90	105.986(4)
γ/°	90	90	90
Volume/Å^3	4033.9(2)	4227.6(3)	37208(3)
Z	4	4	4
ρ_{calc} g/cm^3	1.424	1.585	1.733
μ/mm^{-1}	3.474	3.576	4.267
F(000)	1736.0	2016.0	1908.0
Crystal size/mm^3	0.26 × 0.23 × 0.07	0.324 × 0.268 × 0.219	0.38 × 0.181 × 0.07
2Θ range for data collection/°	5.87 to 52.744	5.932 to 52.742	6.306 to 52.74
Index ranges	-14 ≤ h ≤ 14,	-17 ≤ h ≤ 17,	-16 ≤ h ≤ 16,

	$-27 \le k \le 27$, $-20 \le l \le 18$	$-22 \le k \le 30$, $-15 \le l \le 12$	$-27 \le k \le 25$, $-16 \le l \le 16$
Reflections collected	34525	18282	38292
Independent reflections	8223 [R_{int} = 0.0338, R_{sigma} = 0.0287]	4410 [R_{int} = 0.0325, R_{sigma} = 0.0273]	7581 [R_{int} = 0.0441, R_{sigma} = 0.0294]
Data/restraints/parameters	8223/519/462	4410/0/251	7581/0/407
Goodness-of-fit on F^2	1.218	0.763	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0397, wR_2 = 0.1039	R_1 = 0.0288, wR_2 = 0.0767	R_1 = 0.0352, wR_2 = 0.0857
Final R indexes [all data]	R_1 = 0.0489, wR_2 = 0.1082	R_1 = 0.0351, wR_2 = 0.0855	R_1 = 0.0414, wR_2 = 0.0899
Largest diff. peak/hole / e $Å^{-3}$	1.90/-1.01	1.39/-0.80	1.42/-0.74

Table S2. Bond lengths for the molecular structure of complex **3**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	Cl2	2.4031(14)	C35	C36	1.496(10)
Ir1	Cl1	2.4274(14)	C10	C8	1.436(8)
Ir1	C1	2.060(5)	C8	C6	1.420(7)
Ir1	C16	2.147(6)	C8	C9	1.393(8)
Ir1	C15	2.134(6)	C6	C25	1.422(8)
Ir1	C17	2.226(6)	C6	C4	1.430(7)
Ir1	C34	2.236(6)	C22	C3	1.374(7)
Ir1	C35	2.155(6)	C22	C23	1.441(7)
C1	N1	1.351(7)	C25	C23	1.428(7)
C1	N2	1.361(7)	C3	C4	1.434(7)
N1	C3	1.389(6)	C24	C23	1.395(8)
N1	C2	1.466(7)	C4	C5	1.396(8)
N2	C21	1.457(7)	C7	C5	1.389(8)
N2	C22	1.402(6)	C7	C9	1.381(8)
C16	C15	1.427(10)	C7	C11	1.540(9)
C16	C17	1.435(9)	C30	C32	1.529(12)
C16	C19	1.492(10)	C30	C33	1.524(10)
C26	C27	1.385(9)	C30	C31	1.518(12)
C26	C24	1.396(8)	C11	C13	1.495(13)
C26	C30	1.534(9)	C11	C12	1.510(16)
C15	C35	1.435(9)	C11	C14	1.533(14)
C15	C18	1.492(9)	C11	C14A	1.550(12)
C17	C34	1.398(9)	C11	C13A	1.554(12)
C17	C20	1.500(9)	C11	C12A	1.469(13)
C29	C28	1.429(8)	C44	C43	1.5419
C29	C10	1.351(9)	C39	C38	1.2653
C34	C35	1.443(9)	C39	C40	1.5052
C34	C37	1.493(9)	C43	C42	1.4371
C28	C27	1.405(8)	C42	C41	1.8983
C28	C25	1.414(7)	C40	C41	1.9618

Table S3. Bond angles for the molecular structure of complex **3**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	Ir1	Cl1	85.76(5)	C35	C34	C37	124.5(6)
C1	Ir1	Cl2	92.29(17)	C37	C34	Ir1	126.4(5)
C1	Ir1	Cl1	92.86(18)	C27	C28	C29	121.3(5)
C1	Ir1	C16	111.9(2)	C27	C28	C25	119.4(5)
C1	Ir1	C15	92.0(2)	C25	C28	C29	119.2(5)
C1	Ir1	C17	150.1(2)	C15	C35	Ir1	69.7(3)
C1	Ir1	C34	147.8(2)	C15	C35	C34	107.1(6)
C1	Ir1	C35	109.6(2)	C15	C35	C36	126.6(6)
C16	Ir1	Cl2	154.84(17)	C34	C35	Ir1	73.9(3)
C16	Ir1	Cl1	99.41(19)	C34	C35	C36	125.5(7)
C16	Ir1	C17	38.3(2)	C36	C35	Ir1	129.9(5)
C16	Ir1	C34	63.3(2)	C29	C10	C8	121.2(5)
C16	Ir1	C35	65.1(3)	C26	C27	C28	122.2(5)
C15	Ir1	Cl2	138.1(2)	C6	C8	C10	118.6(5)
C15	Ir1	Cl1	135.5(2)	C9	C8	C10	121.1(5)
C15	Ir1	C16	38.9(3)	C9	C8	C6	120.3(5)
C15	Ir1	C17	64.0(2)	C8	C6	C25	120.0(5)
C15	Ir1	C34	63.9(2)	C8	C6	C4	117.8(5)
C15	Ir1	C35	39.1(3)	C25	C6	C4	122.2(5)
C17	Ir1	Cl2	117.35(17)	N2	C22	C23	130.8(5)
C17	Ir1	Cl1	92.86(18)	C3	C22	N2	106.1(4)
C17	Ir1	C34	36.5(2)	C3	C22	C23	123.0(5)
C34	Ir1	Cl2	92.61(17)	C28	C25	C6	119.8(5)
C34	Ir1	Cl1	119.24(17)	C28	C25	C23	118.7(5)
C35	Ir1	Cl2	101.06(18)	C6	C25	C23	121.6(5)
C35	Ir1	Cl1	156.05(17)	N1	C3	C4	130.9(5)
C35	Ir1	C17	63.5(2)	C22	C3	N1	106.4(4)
C35	Ir1	C34	38.3(2)	C22	C3	C4	122.6(5)
N1	C1	Ir1	126.2(4)	C23	C24	C26	122.3(5)
N1	C1	N2	105.3(4)	C6	C4	C3	114.9(5)
N2	C1	Ir1	126.0(4)	C5	C4	C6	119.2(5)
C1	N1	C3	111.5(4)	C5	C4	C3	125.8(5)
C1	N1	C2	124.0(4)	C5	C7	C11	119.6(5)
C3	N1	C2	124.5(4)	C9	C7	C5	118.2(5)
C1	N2	C21	125.2(4)	C9	C7	C11	122.1(5)
C1	N2	C22	110.7(4)	C32	C30	C26	109.2(7)
C22	N2	C21	124.0(4)	C33	C30	C26	112.3(5)
C15	C16	Ir1	70.0(3)	C33	C30	C32	107.7(7)
C15	C16	C17	107.7(6)	C31	C30	C26	109.0(6)
C15	C16	C19	127.2(7)	C31	C30	C32	110.6(7)
C17	C16	Ir1	73.8(4)	C31	C30	C33	108.0(8)
C17	C16	C19	124.4(7)	C25	C23	C22	114.9(5)
C19	C16	Ir1	128.9(5)	C24	C23	C22	125.8(5)
C27	C26	C24	117.9(5)	C24	C23	C25	119.3(5)
C27	C26	C30	120.0(5)	C7	C5	C4	122.4(5)
C24	C26	C30	122.0(6)	C7	C9	C8	121.9(5)
C16	C15	Ir1	71.0(4)	C7	C11	C14A	107.5(6)
C16	C15	C35	108.0(6)	C7	C11	C13A	109.5(6)
C16	C15	C18	127.0(7)	C13	C11	C7	113.5(7)
C35	C15	Ir1	71.2(3)	C13	C11	C12	108.5(10)

C35	C15	C18	124.9(7)	C13	C11	C14	109.5(9)
C18	C15	Ir1	125.5(5)	C12	C11	C7	109.2(7)
C16	C17	Ir1	67.9(3)	C12	C11	C14	106.6(10)
C16	C17	C20	124.8(7)	C14	C11	C7	109.3(7)
C34	C17	Ir1	72.1(3)	C14A	C11	C13A	103.6(7)
C34	C17	C16	108.5(6)	C12A	C11	C7	114.6(6)
C34	C17	C20	126.6(6)	C12A	C11	C14A	109.5(8)
C20	C17	Ir1	127.0(5)	C12A	C11	C13A	111.5(6)
C10	C29	C28	121.1(5)	C38	C39	C40	150.2
C17	C34	Ir1	71.4(3)	C42	C43	C44	137.6
C17	C34	C35	108.6(5)	C43	C42	C41	85.2
C17	C34	C37	126.9(6)	C39	C40	C41	102.4
C35	C34	Ir1	67.8(3)	C42	C41	C40	171.4

Table S4. Bond lengths for the molecular structure of complex **4**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	O2[1]	2.100(3)	C7	C11	1.531(5)
Ir1	O2	2.100(3)	C18	C15	1.502(8)
Ir1	C1	2.038(5)	C16	C17	1.454(6)
Ir1	C21	2.562(6)	C16	C15	1.427(5)
Ir1	C16	2.144(4)	C16	C19	1.506(6)
Ir1	C16[1]	2.144(4)	C6	C6[1]	1.432(7)
Ir1	C17	2.232(4)	C6	C8	1.427(5)
Ir1	C17[1]	2.232(4)	C6	C4	1.424(5)
Ir1	C15	2.144(5)	C10	C10[1]	1.339(8)
Cl1	C22	1.736(5)	C10	C8	1.439(5)
Cl3	C22	1.758(5)	C8	C9	1.392(5)
O2	C21	1.326(4)	C5	C4	1.400(5)
N1	C1	1.354(4)	C11	C14	1.534(6)
N1	C2	1.460(4)	C11	C12	1.539(6)
N1	C3	1.397(4)	C3	C3[1]	1.379(7)
C1	N1[1]	1.354(4)	C3	C4	1.439(5)
O1	C21	1.220(7)	C17	C17[1]	1.392(10)
C21	O2[1]	1.326(4)	C17	C20	1.503(6)
C13	C11	1.541(7)	C22	Cl2	1.738(5)
C7	C9	1.390(5)	C15	C16[1]	1.427(5)
C7	C5	1.397(5)			

[1]+X,3/2-Y,+Z

Table S5. Bond angles for the molecular structure of complex **4**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2[1]	Ir1	O2	62.16(16)	O1	C21	O2[1]	125.2(2)
O2[1]	Ir1	C21	31.09(8)	O1	C21	O2	125.2(2)
O2	Ir1	C21	31.08(8)	C9	C7	C5	118.0(3)
O2[1]	Ir1	C16	112.65(13)	C9	C7	C11	120.1(3)
O2	Ir1	C16	160.00(14)	C5	C7	C11	121.8(4)
O2	Ir1	C16[1]	112.65(14)	C17	C16	Ir1	73.9(2)
O2[1]	Ir1	C16[1]	160.00(14)	C17	C16	C19	124.8(4)
O2	Ir1	C17[1]	101.52(14)	C15	C16	Ir1	70.6(3)

O2[1]	Ir1	C17	101.52(14)	C15	C16	C17	107.8(4)
O2	Ir1	C17	121.45(13)	C15	C16	C19	126.7(4)
O2[1]	Ir1	C17[1]	121.45(13)	C19	C16	Ir1	128.6(3)
O2[1]	Ir1	C15	148.91(8)	C8	C6	C6[1]	119.7(2)
O2	Ir1	C15	148.91(8)	C4	C6	C6[1]	122.0(2)
C1	Ir1	O2[1]	84.94(14)	C4	C6	C8	118.2(3)
C1	Ir1	O2	84.94(14)	C10[1]	C10	C8	121.6(2)
C1	Ir1	C21	83.47(19)	C6	C8	C10	118.6(3)
C1	Ir1	C16[1]	114.49(16)	C9	C8	C6	120.1(3)
C1	Ir1	C16	114.49(16)	C9	C8	C10	121.2(3)
C1	Ir1	C17	152.94(16)	C7	C9	C8	121.9(3)
C1	Ir1	C17[1]	152.94(16)	C7	C5	C4	122.4(4)
C1	Ir1	C15	96.8(2)	C7	C11	C13	109.0(4)
C16[1]	Ir1	C21	140.98(12)	C7	C11	C14	111.9(3)
C16	Ir1	C21	140.98(13)	C7	C11	C12	108.9(4)
C16[1]	Ir1	C16	65.0(2)	C14	C11	C13	109.3(4)
C16	Ir1	C17[1]	63.58(16)	C14	C11	C12	108.4(4)
C16[1]	Ir1	C17[1]	38.74(16)	C12	C11	C13	109.3(4)
C16	Ir1	C17	38.74(16)	N1	C3	C4	130.6(3)
C16[1]	Ir1	C17	63.59(16)	C3[1]	C3	N1	106.35(19)
C16[1]	Ir1	C15	38.86(13)	C3[1]	C3	C4	122.9(2)
C16	Ir1	C15	38.86(13)	C16	C17	Ir1	67.3(2)
C17	Ir1	C21	115.49(16)	C16	C17	C20	124.1(5)
C17[1]	Ir1	C21	115.49(16)	C17[1]	C17	Ir1	71.83(13)
C17	Ir1	C17[1]	36.3(3)	C17[1]	C17	C16	108.3(2)
C15	Ir1	C21	179.71(18)	C17[1]	C17	C20	127.6(3)
C15	Ir1	C17	64.24(17)	C20	C17	Ir1	124.5(3)
C15	Ir1	C17[1]	64.23(17)	Cl1	C22	Cl3	110.9(3)
C21	O2	Ir1	94.1(3)	Cl1	C22	Cl2	111.0(3)
C1	N1	C2	123.2(3)	Cl2	C22	Cl3	108.4(3)
C1	N1	C3	110.5(3)	C6	C4	C3	114.9(3)
C3	N1	C2	126.1(3)	C5	C4	C6	119.3(3)
N1[1]	C1	Ir1	126.9(2)	C5	C4	C3	125.8(3)
N1	C1	Ir1	126.9(2)	C18	C15	Ir1	123.4(4)
N1[1]	C1	N1	106.2(4)	C16	C15	Ir1	70.6(3)
O2[1]	C21	Ir1	54.9(2)	C16[1]	C15	Ir1	70.6(3)
O2	C21	Ir1	54.9(2)	C16[1]	C15	C18	126.2(2)
O2	C21	O2[1]	109.7(5)	C16	C15	C18	126.2(2)
O1	C21	Ir1	177.4(4)	C16	C15	C16[1]	107.7(5)

[1]+X,3/2-Y,+Z

Table S6. Bond lengths for the molecular structure of complex **6**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ir1	C1	2.028(4)	O1	C29	1.230(6)
Ir1	O3	2.113(3)	C20	C19	1.397(8)
Ir1	C20	2.205(5)	C20	C21	1.444(8)
Ir1	C29	2.540(5)	C20	C25	1.494(8)
Ir1	C19	2.200(5)	C24	C19	1.511(8)
Ir1	C18	2.154(5)	C8	C5	1.436(6)
Ir1	C21	2.143(5)	C8	C12	1.425(5)
Ir1	O2	2.096(3)	C8	C9	1.406(6)

Ir1	C22	2.140(5)	C29	O2	1.328(6)
Cl2	C30	1.728(7)	C4	C5	1.365(6)
Cl4	C32	1.747(6)	C4	C7[1]	1.437(5)
Cl3	C30	1.740(7)	C19	C18	1.423(8)
Cl1	C30	1.749(8)	C17	C14	1.521(7)
Cl5	C32	1.735(6)	C12	C12[1]	1.438(7)
Cl8	C31	1.728(8)	C12	C7	1.426(6)
Cl7	C31	1.723(8)	C7	C4[1]	1.437(5)
Cl6	C32	1.741(7)	C7	C6	1.403(6)
Cl9	C31	1.747(8)	C13	C14	1.535(6)
C1	N2	1.364(5)	C13	C9	1.379(6)
C1	N1	1.358(6)	C13	C6	1.387(6)
N2	C4	1.394(5)	C14	C16	1.536(8)
N2	C3	1.458(5)	C14	C15	1.499(7)
O3	C29	1.301(6)	C18	C22	1.401(8)
N1	C5	1.400(5)	C18	C23	1.520(8)
N1	C2	1.470(5)	C21	C22	1.423(8)
C27	C22	1.512(8)	C21	C26	1.501(8)

[1]-X,1-Y,-Z

Table S7. Bond angles for the molecular structure of complex **6**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Ir1	O3	85.48(16)	O1	C29	O2	123.3(5)
C1	Ir1	C20	159.2(2)	O2	C29	Ir1	55.5(2)
C1	Ir1	C29	84.89(17)	N2	C4	C7[1]	130.5(4)
C1	Ir1	C19	145.5(2)	C5	C4	N2	106.7(3)
C1	Ir1	C18	109.2(2)	C5	C4	C7[1]	122.6(4)
C1	Ir1	C21	120.5(2)	C20	C19	Ir1	71.7(3)
C1	Ir1	O2	85.65(16)	C20	C19	C24	127.6(6)
C1	Ir1	C22	97.8(2)	C20	C19	C18	109.4(5)
O3	Ir1	C20	102.29(16)	C24	C19	Ir1	124.8(4)
O3	Ir1	C29	30.76(14)	C18	C19	Ir1	69.2(3)
O3	Ir1	C19	127.61(18)	C18	C19	C24	123.1(6)
O3	Ir1	C18	165.28(18)	N1	C5	C8	130.9(4)
O3	Ir1	C21	108.02(18)	C4	C5	N1	106.6(3)
O3	Ir1	C22	142.02(19)	C4	C5	C8	122.5(4)
C20	Ir1	C29	111.69(17)	C8	C12	C12[1]	121.1(4)
C19	Ir1	C20	37.0(2)	C8	C12	C7	117.6(3)
C19	Ir1	C29	117.79(18)	C7	C12	C12[1]	121.3(4)
C18	Ir1	C20	63.7(2)	C12	C7	C4[1]	116.0(3)
C18	Ir1	C29	147.3(2)	C6	C7	C4[1]	124.1(4)
C18	Ir1	C19	38.1(2)	C6	C7	C12	119.8(4)
C21	Ir1	C20	38.8(2)	C9	C13	C14	122.4(4)
C21	Ir1	C29	133.97(19)	C9	C13	C6	118.1(4)
C21	Ir1	C19	63.47(19)	C6	C13	C14	119.4(4)
C21	Ir1	C18	64.5(2)	C17	C14	C13	109.2(4)
O2	Ir1	O3	62.25(13)	C17	C14	C16	108.2(5)
O2	Ir1	C20	115.11(17)	C13	C14	C16	109.3(4)
O2	Ir1	C29	31.49(14)	C15	C14	C17	110.4(5)
O2	Ir1	C19	100.68(17)	C15	C14	C13	112.1(4)
O2	Ir1	C18	117.98(19)	C15	C14	C16	107.6(5)

O2	Ir1	C21	152.42(19)	C13	C9	C8	122.3(4)
O2	Ir1	C22	155.51(19)	C19	C18	Ir1	72.7(3)
C22	Ir1	C20	64.2(2)	C19	C18	C23	125.7(6)
C22	Ir1	C29	172.4(2)	C22	C18	Ir1	70.4(3)
C22	Ir1	C19	63.3(2)	C22	C18	C19	107.6(5)
C22	Ir1	C18	38.1(2)	C22	C18	C23	125.8(6)
C22	Ir1	C21	38.8(2)	C23	C18	Ir1	131.0(4)
N2	C1	Ir1	126.9(3)	Cl5	C32	Cl4	109.1(3)
N1	C1	Ir1	127.6(3)	Cl5	C32	Cl6	109.8(3)
N1	C1	N2	105.4(3)	Cl6	C32	Cl4	111.5(3)
C1	N2	C4	110.6(3)	C13	C6	C7	122.2(4)
C1	N2	C3	122.2(4)	C20	C21	Ir1	73.0(3)
C4	N2	C3	127.0(3)	C20	C21	C26	124.1(6)
C29	O3	Ir1	93.1(3)	C22	C21	Ir1	70.5(3)
C1	N1	C5	110.6(3)	C22	C21	C20	107.4(5)
C1	N1	C2	122.5(4)	C22	C21	C26	128.2(6)
C5	N1	C2	126.6(4)	C26	C21	Ir1	127.3(4)
C19	C20	Ir1	71.3(3)	C29	O2	Ir1	93.0(3)
C19	C20	C21	107.1(5)	C27	C22	Ir1	125.1(4)
C19	C20	C25	126.1(6)	C18	C22	Ir1	71.5(3)
C21	C20	Ir1	68.3(3)	C18	C22	C27	125.0(6)
C21	C20	C25	126.8(6)	C18	C22	C21	108.6(5)
C25	C20	Ir1	126.2(4)	C21	C22	Ir1	70.7(3)
C12	C8	C5	116.1(3)	C21	C22	C27	126.4(6)
C9	C8	C5	124.0(4)	Cl8	C31	Cl9	108.1(4)
C9	C8	C12	119.8(4)	Cl7	C31	Cl8	109.5(4)
O3	C29	Ir1	56.2(2)	Cl7	C31	Cl9	111.5(5)
O3	C29	O2	111.7(4)	Cl2	C30	Cl3	110.1(4)
O1	C29	Ir1	178.7(4)	Cl2	C30	Cl1	113.6(5)
O1	C29	O3	125.0(5)	Cl3	C30	Cl1	110.0(4)

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3. References

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