Supplementary Material (ESI) for Dalton Transactions
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Supporting Information

Near-infrared emitting iridium(III) complexes for mitochondrial imaging in living cells

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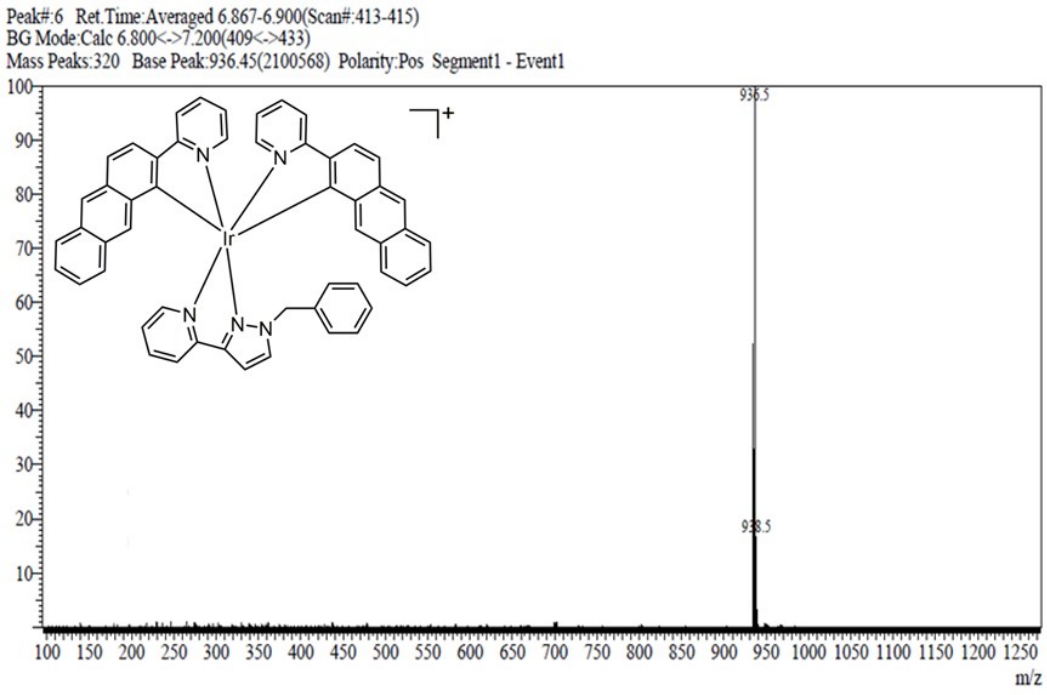

Fig. S1 ESI-MS spectrum of **Ir1**

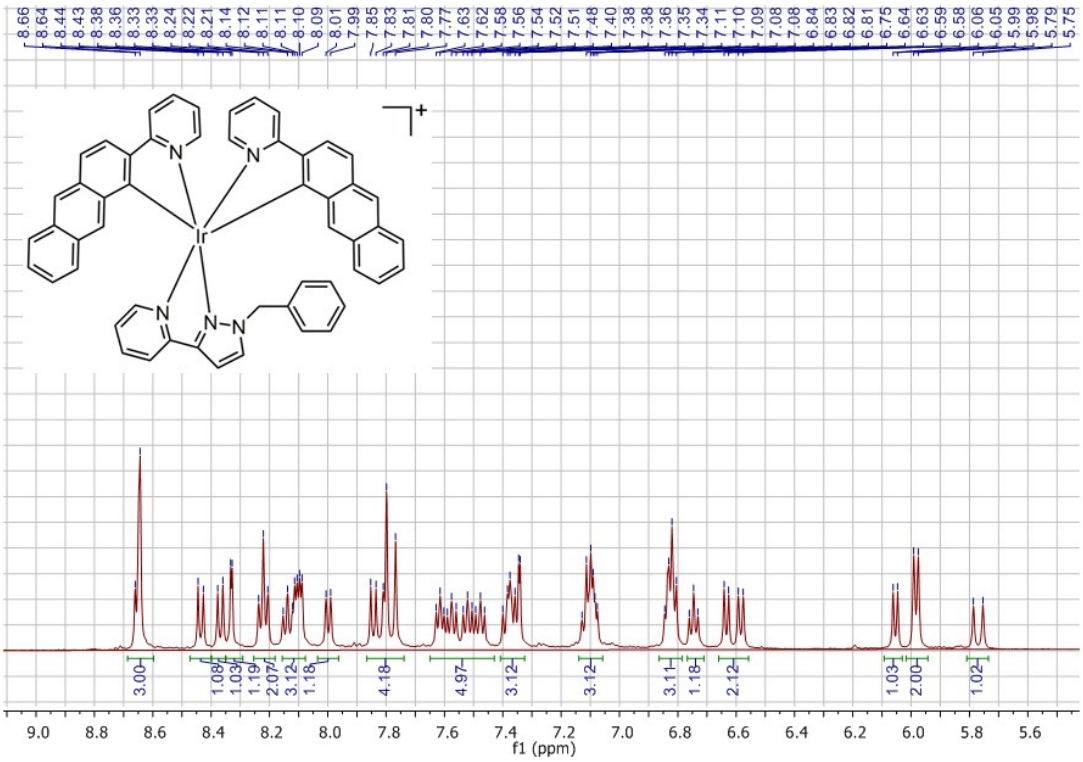

Fig. S2 ^{1}H NMR spectrum of **Ir1**

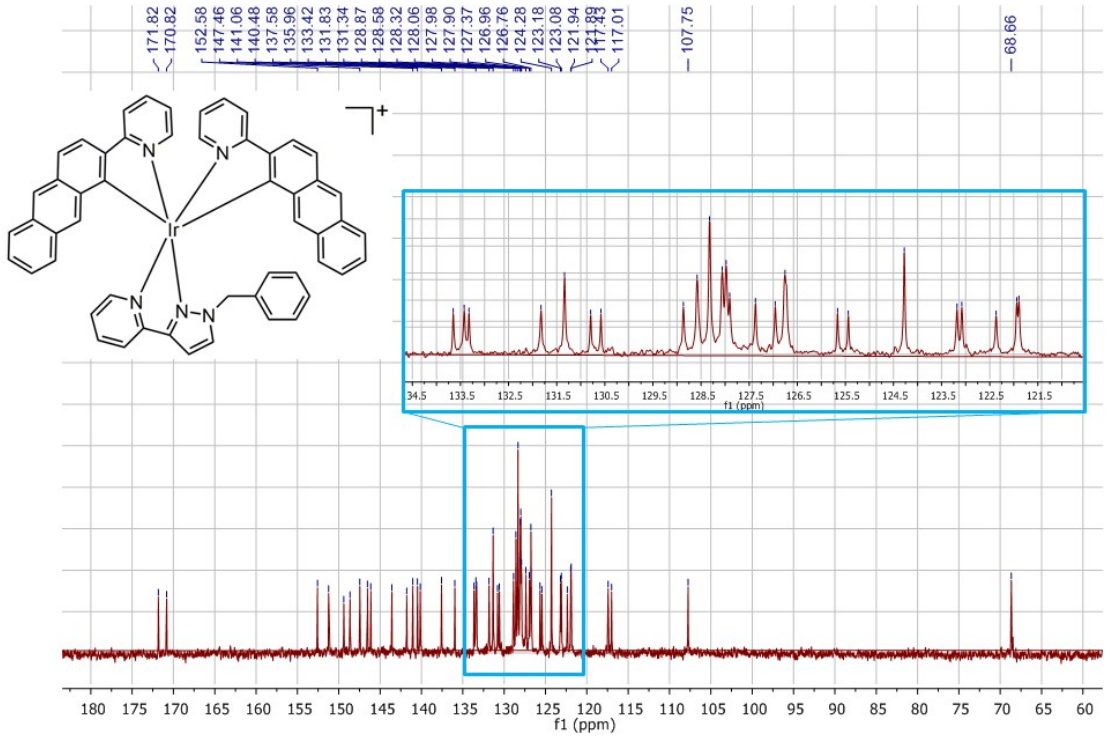

Fig. S3 ^{13}C NMR spectrum of **Ir1**

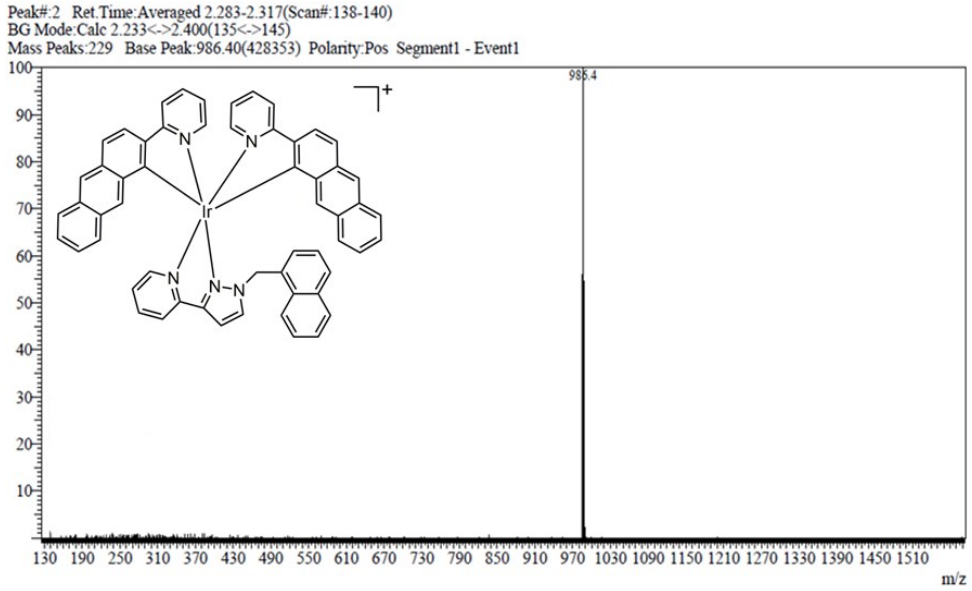

Fig. S4 ESI-MS spectrum of **Ir2**

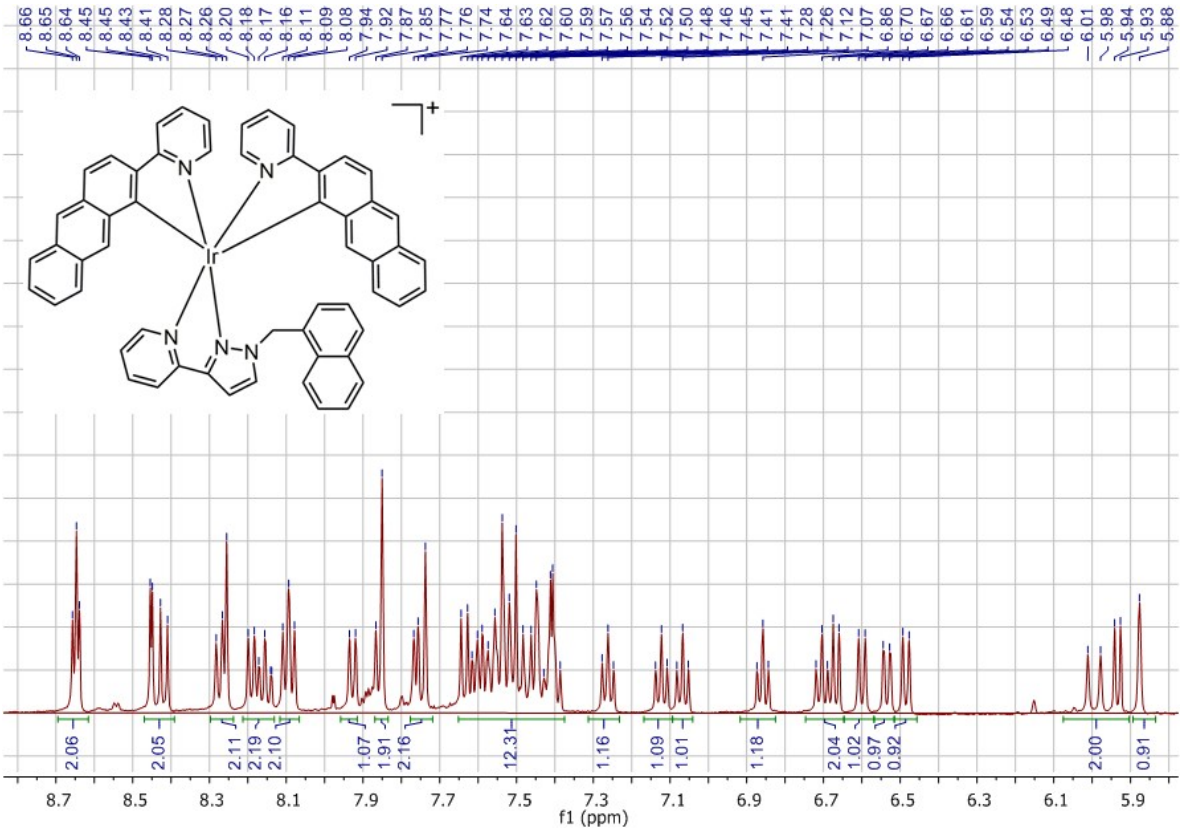

Fig. S5 ^{1}H NMR spectrum of **Ir2**

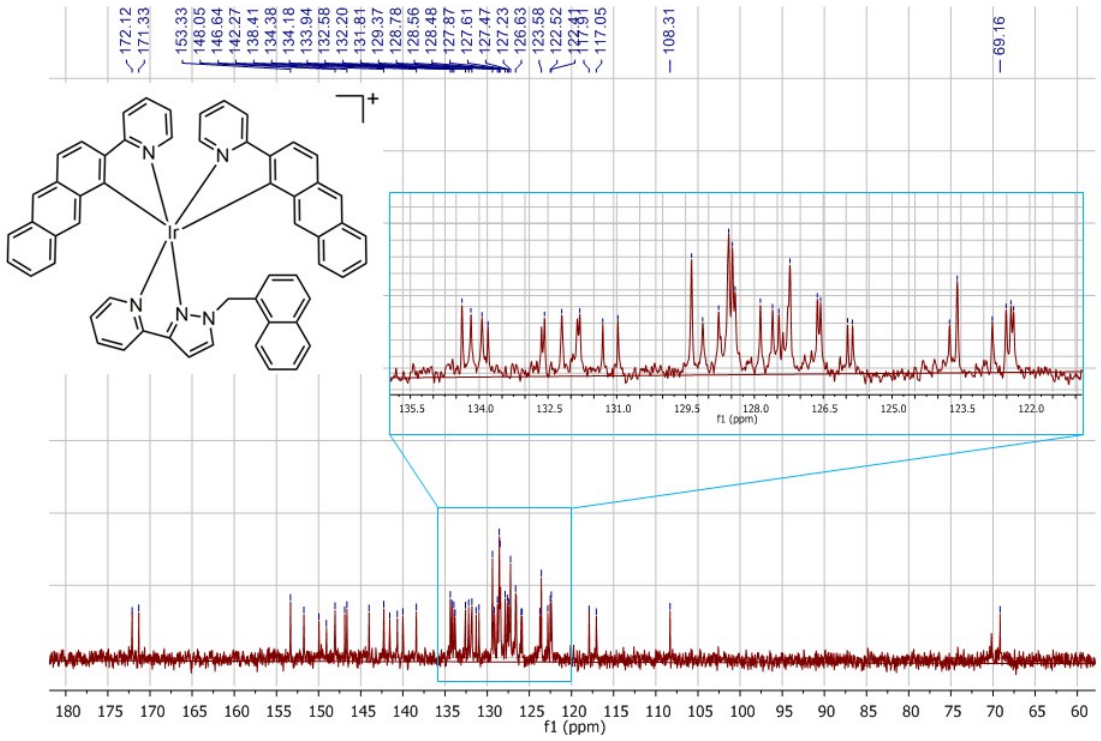

Fig. S6 ^{13}C NMR spectrum of **Ir2**

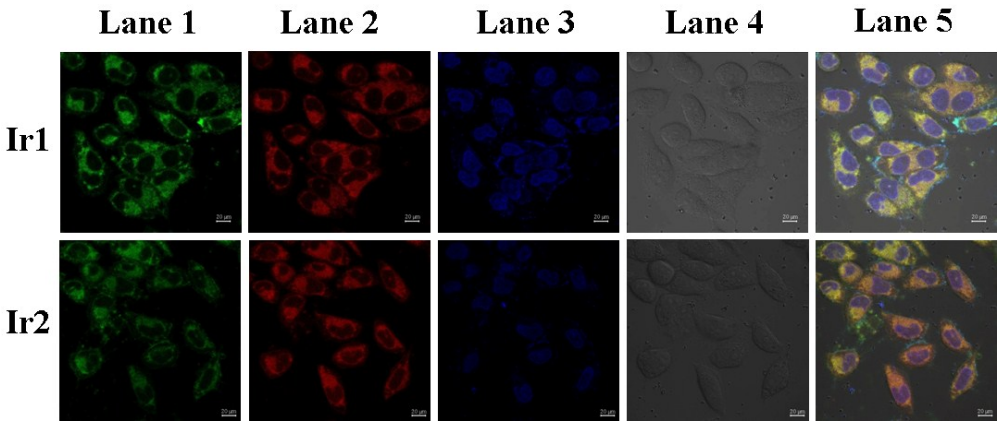

Fig. S7 Confocal phosphorescence images, bright field images and their overlay of living HeLa cells incubated with 20 μM of **Ir1**–**Ir2** in PBS (pH = 7.4) for 1 h at 37 °C, followed by 50 *n*M of MTG and 2 μg/mL of DAPI, respectively. lane 1, confocal phosphorescence images of MTG; lane 2, confocal phosphorescence images of **Ir1**–**Ir2**; lane 3, confocal phosphorescence images of DAPI; lane 4, bright field images; lane 5, overlay of lane 1, lane 2, lane 3, lane 4 and lane 5.

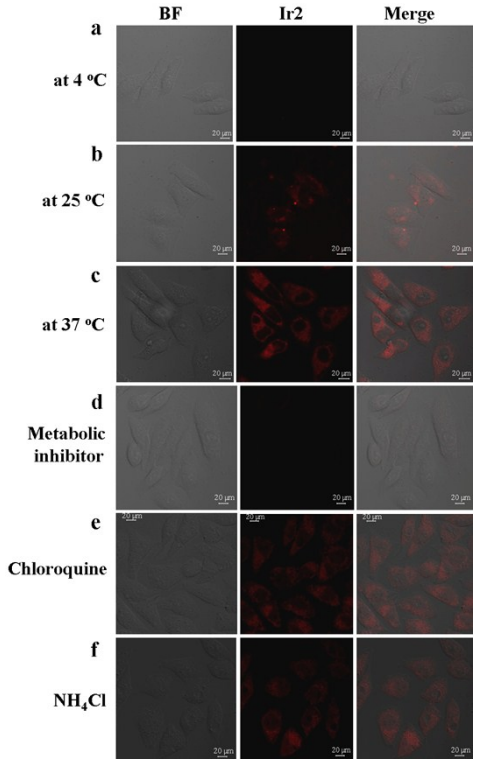

Fig. S8 Confocal phosphorescence images and bright-field images of living HeLa cells incubated with 20 μM **Ir2** in PBS (pH = 7.4) under different conditions. (a) The cells were incubated with 20 μM of **Ir2** at 4 °C for 1 h. (b) The cells were incubated with 20 μM of **Ir2** at 25 °C for 1 h. (c) The cells were incubated with 20 μM of **Ir2** at 37 °C for 1 h. (d) The cells were preincubated with 50 *m*M 2-deoxy-D-glucose and 5 μM oligomycin in PBS for 1 h at 37 °C and then incubated with 20 μM of **Ir2** at 37 °C for 1 h. (e and f) The cells were pretreated with endocytic inhibitors chloroquine (100 μM) and NH_4Cl (50 *m*M), respectively, and then incubated with 20 μM of **Ir2** at 37 °C for 1 h.

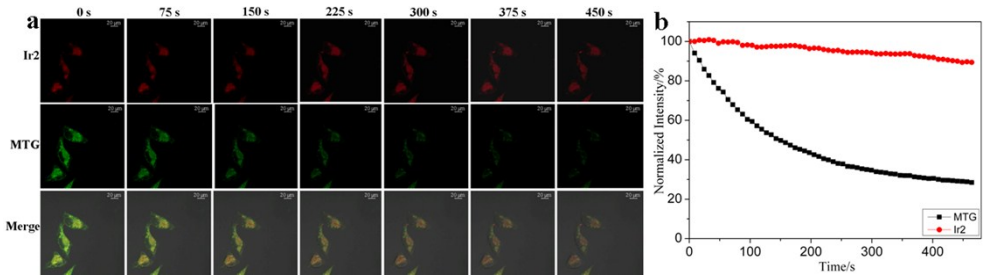

Fig. S9 The anti-bleaching properties of **Ir2**. HeLa cells were treated with 20 μM of **Ir2**, followed by 50 *n*M of MTG. (a) Confocal phosphorescence images of cells stained with **Ir2** and MTG with an increasing bleaching time (450 s). (b) Intensity loss (%) of the phosphorescence of

Ir2 and MTG with an increasing bleaching time.

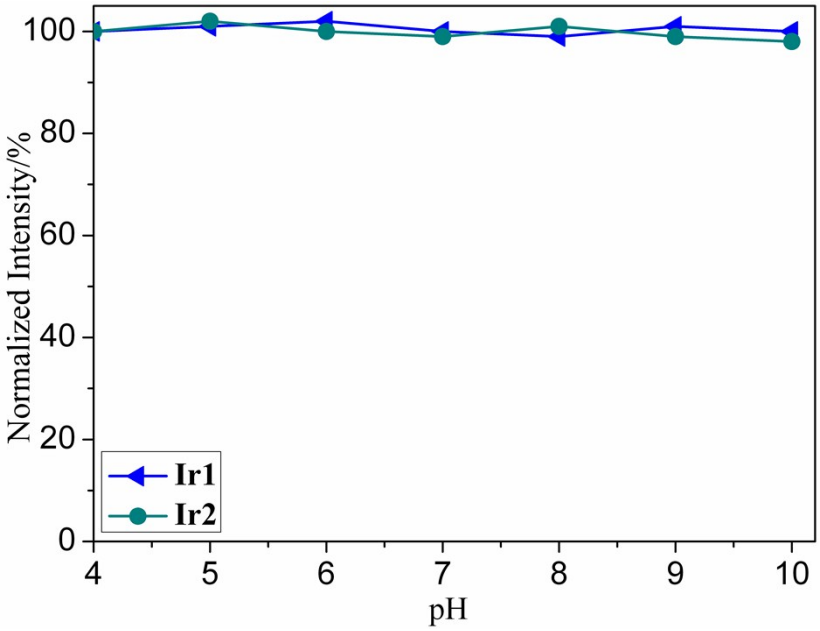

Fig. S10 The emission intensity of 10 μM of **Ir1**–**Ir2** at 751 and 750 nm, respectively, under different pH in Britton-Robinson buffer.

Table S1 Crystal data and structure refinement for **Ir1**

Identification code	**Ir1**
Empirical formula	$C_{53}H_{37}ClN_5Ir$
Formula weight	971.52
Temperature/K	150(2)
Crystal system	Monoclinic
Space group	C1 2/c 1
a/Å	33.9838(13)
b/Å	13.9225(6)
c/Å	24.0406(11)
α/°	90
β/°	129.3560(10)
γ/°	90
Volume/Å3	8795.0(7)
Z	8
ρ_{calc}/g cm^{-3}	1.467
μ/mm^{-1}	3.139
F(000)	3872
Crystal size/mm^3	0.31 × 0.25 × 0.14
Radiation	Mo-K□ (λ = 0.71073)

2θ range for data collection/°	4.48 to 52.74
Index ranges	$-42 \le h \le 42$, $-17 \le k \le 17$, $-30 \le l \le 30$
Reflections collected	8952
Independent reflections	7593 [R_{int} = 0.0344, R_{unet} = 0.0270]
Data/restraints/parameters	8952/1/541
Goodness-of-fit on F^2	1.105
Final R indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0340, wR_2 = 0.0980
Final R indexes [all data]	R_1 = 0.0413, wR_2 = 0.1013

Table S2 Selected bond lengths (Å) and angles (°) for **Ir1**

Ir1-N1	2.012(4)	N1-Ir1-N3	174.1(1)	C30-Ir1-N4	102.2(1)
Ir1-C11	2.115(3)	N1-Ir1-C30	92.7(2)	N2-Ir1-N1	87.7(2)
Ir1-N3	2.201(4)	N1-Ir1-N4	103.4(2)	N2-Ir1-C11	91.8(2)
Ir1-C30	2.099(3)	C11-Ir1-N3	106(1)	N2-Ir1-N3	94.8(2)
Ir1-N2	1.995(4)	C11-Ir1-N4	87.7(1)	N2-Ir1-C30	79.6(2)
Ir1-N4	2.188(3)	C30-Ir1-C11	168.5(1)	N2-Ir1-N4	168.6(2)
N1-Ir1-C11	79.2(2)	C30-Ir1-N3	82.6(1)	N4-Ir1-N3	74.4(1)

Table S3 Absorption and photoluminescence data of **Ir1**-**Ir2**.

Complex	λ_{abs} /nm					λ_{PL} /nm	τ/ns	Φ_{PL}
Ir1	225	316	386	440	500	751	442	0.62
Ir2	225	316	386	440	500	750	456	0.85