Supporting Information

Photoluminescence and electroluminescence of deep red iridium(III) complexes with 2,3-diphenylquinoxaline derivatives and 1,3,4-oxadiazole derivatives ligands

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Table S1. Parameters associated with the single crystal diffraction data collection for **Ir1** and **Ir3**.

	Ir1	**Ir3**
Formula	$C_{54}H_{35}IrN_6O_2$	$C_{54}H_{31}F_4IrN_6O_2$
Formula weight	992.08	1064.05
T (K)	293(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$C2/c$
a (Å)	11.3469(19)	29.928(10)
b (Å)	31.314(5)	18.643(6)
c (Å)	13.335(2)	22.998(2)
α (deg)	90	90
β (deg)	110.451(3)	135.639(5)
γ (deg)	90	90
V (Å^3)	4439.4(13)	8972(5)
Z	4	8
ρ_{calcd} (g/cm^3)	1.484	1.575
μ (Mo Kα) (mm^{-1})	3.057	3.043
F (000)	1976	4208
Range of transm factors (deg)	1.755-25.009	1.463-27.761
Reflns collected	24108	30648
Unique(R_{int})	7779(0.0657)	10389(0.0696)
$R_1{}^a$, $wR_2{}^b$ [I > 2s(I)]	0.1040, 0.2567	0.0393, 0.0670
$R_1{}^a$, $wR_2{}^b$ (all data)	0.1210, 0.2655	0.0755, 0.0778
GOF on F^2	1.133	0.930
CCDC number	1535471	1535473

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma F_o|$. $wR_2{}^b = [\Sigma w(F_o{}^2 - F_c{}^2)^2/\Sigma w(F_o{}^2)]^{1/2}$

GOF = $[(\Sigma w|F_o| - |F_c|)^2/(N_{obs} - N_{param})]^{1/2}$.

Table S2. The table of selected bond lengths and angles of **Ir1** and **Ir3**.

	Ir1	**Ir3**
Selected bonds	Bond length (Å)	Bond length (Å)
Ir(1)-C(1)	1.976(19)	1.985(4)
Ir(1)-C(21)	1.977(18)	1.992(5)
Ir(1)-N(1)	2.087(17)	2.069(3)
Ir(1)-N(3)	2.061(11)	2.068(4)
Ir(1)-N(5)	2.159(15)	2.139(4)
Ir(1)-O(1)	2.181(12)	2.148(3)
Selected angles	(°)	(°)
C(1)-Ir(1)-C(21)	91.2(7)	93.22(17)
C(1)-Ir(1)-N(1)	80.5(7)	79.50(16)
C(1)-Ir(1)-N(3)	99.8(6)	101.18(16)
C(1)-Ir(1)-N(5)	171.2(7)	171.78(15)
C(1)-Ir(1)-O(1)	88.3(6)	87.09(15)
C(21)-Ir(1)-N(1)	99.7(7)	94.69(16)
C(21)-Ir(1)-N(3)	79.4(6)	80.30(16)
C(21)-Ir(1)-N(5)	96.7(7)	95.00(15)
C(21)-Ir(1)-O(1)	178.8(7)	179.59(15)
N(1)-Ir(1)-N(3)	179.0(6)	174.96(14)
N(1)-Ir(1)-N(5)	94.5(6)	98.16(14)
N(1)-Ir(1)-O(1)	79.1(5)	79.13(13)
N(3)-Ir(1)-N(5)	85.3(5)	86.72(14)
N(3)-Ir(1)-O(1)	101.8(4)	100.22(13)
N(5)-Ir(1)-O(1)	83.7(5)	84.68(13)

Table S3. Electrochemical data of **Ir1**, **Ir2**, **Ir3** and **Ir4**.

Complex	E_{ox} (V) [a]	E_{red} (V) [a]	HOMO (eV) [b]	LUMO (eV) [c]	λ_{edge} (nm) [d]	E_g (eV) [e]
Ir1	0.626	-1.82	-5.26	-3.46	689	1.80
Ir2	0.726	-1.73	-5.36	-3.60	704	1.76
Ir3	0.700	-1.80	-5.33	-3.44	656	1.89
Ir4	0.820	-1.65	-5.45	-3.57	660	1.88

[a] Oxidation and reduction potential measured in deaerated dichloromethane at 0.05 V/s, *tetra*-n-butylammonium hexafluorophosphate (0.1 M) was used as the supporting electrolyte.

[b] The HOMO energy levels were calculated from the equation: HOMO (eV) = -(E_{ox} - $E^{+}_{Fc}{}^{+}_{/Fc}$ + 4.8).

[c] The LUMO energy levels were calculated form the equation: LUMO = HOMO + E_g.

[d] UV-vis absorption edge.

[e] The band gap (E_g) was calculated from the equation: $E_g = 1240/\lambda_{edge}$.

Table S4. Percentage distributions of HOMO and LUMO in **Ir1**, **Ir2**, **Ir3** and **Ir4**.

Complex	Orbital	Energy/eV (Calculated)	E_{gap}/eV (Calculated)	Composition (%)		
				Ir	Main ligands	POP
Ir1	HOMO	-5.256	2.772	15.86	8.87	75.27
	LUMO	-2.483		3.64	94.55	1.81
Ir2	HOMO	-5.334	2.728	15.17	8.48	76.35
	LUMO	-2.605		3.69	94.57	1.74
Ir3	HOMO	-5.319	2.787	14.62	8.26	77.12
	LUMO	-2.532		3.47	94.77	1.76
Ir4	HOMO	-5.396	2.743	14.17	8.04	77.79
	LUMO	-2.653		3.51	94.80	1.69

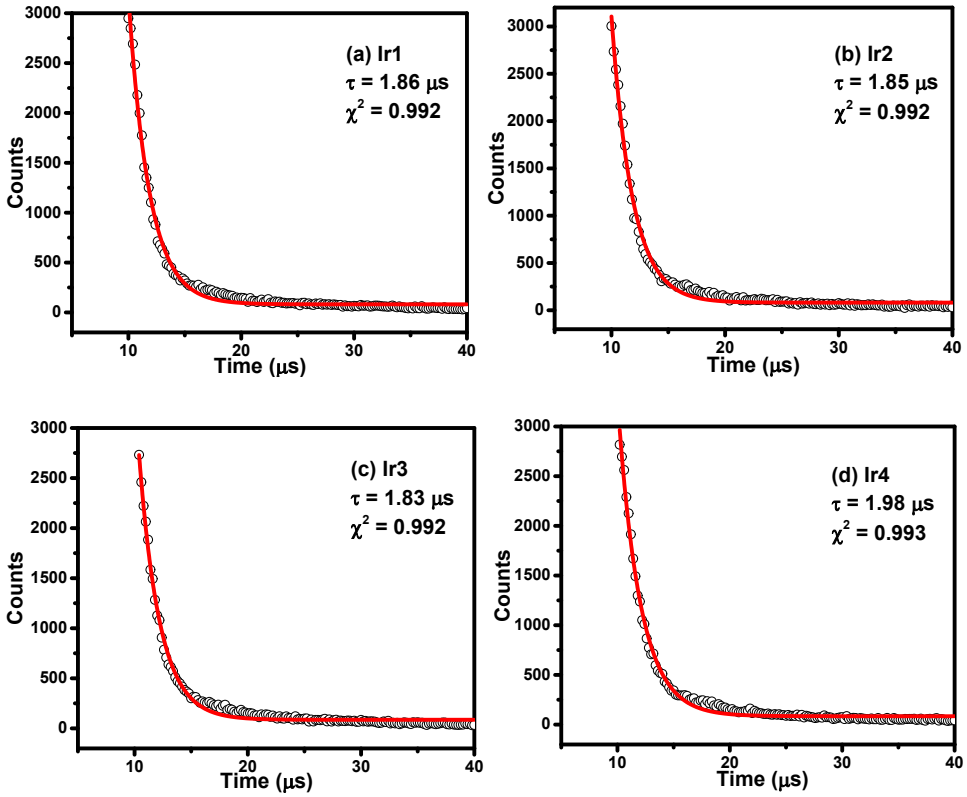

Fig. S1. The lifetime curves of (a) **Ir1**, (b) **Ir2**, (c) **Ir3** and (d) **Ir4** in degassed CH_2Cl_2 solution at a concentration of 5×10^{-5} mol·L^{-1} at room temperature.

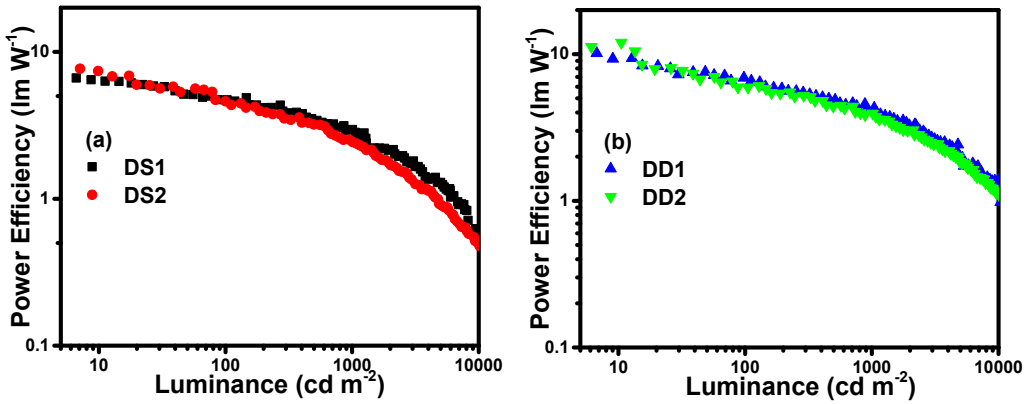

Fig. S2. Power efficiency-luminance (η_p-L) curves of devices (a) **DS1** and **DS2**, (b) **DD1** and **DD2**.

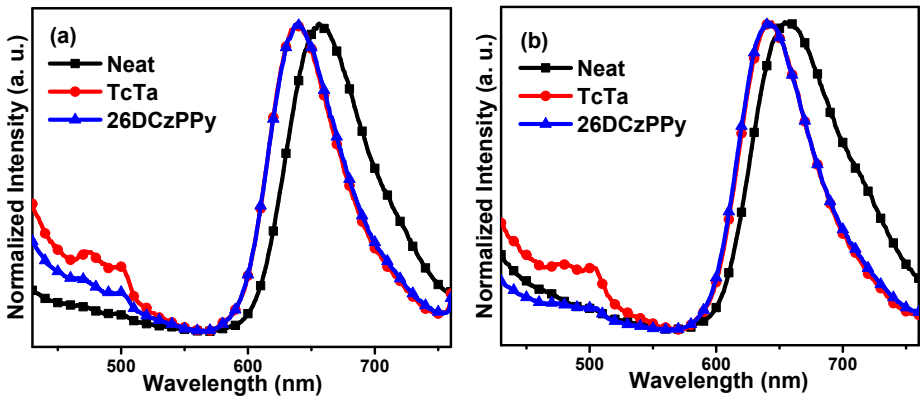

Fig. S3. PL spectra in neat and doped films of (a) **Ir3** and (b) **Ir4**.

Table S5. Photoluminescence data of **Ir3** and **Ir4** in neat and doped films.

Complex	Neat film [a]	2 wt% doped in TcTa [a]	2 wt% doped in 26DCzPPy [a]
Ir3	656 nm	639 nm	639 nm
Ir4	654 nm	644 nm	641 nm

[a] Excitation wavelength 388 nm for **Ir3** and 391 nm for **Ir4**.