Supporting Information

Efficient deep red electroluminescence of iridium(III) complexes with 2,3-diphenylquinoxaline derivatives and tetraphenylimidodiphosphinate

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Table S1. Parameters associated with the single crystal diffraction data collection for **Ir2**, **Ir3** and **Ir4**.

	Ir2	**Ir3**	**Ir4**
Formula	$C_{64}H_{42}F_4IrN_5O_2P_2$	$C_{64}H_{42}F_4IrN_5O_2P_2$	$C_{64}H_{38}F_8IrN_5O_2P_2$
Formula weight	1243.16	1243.16	1315.13
T (K)	296(2)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/n$	$P2_1/c$
a (Å)	10.927(2)	15.0722(14)	12.6583(6)
b (Å)	15.470(3)	15.1646(14)	20.5922(10)
c (Å)	16.813(3)	23.699(2)	21.1398(10)
α (deg)	80.513(4)	90	90
β (deg)	72.599(4)	92.214(2)	95.5170(10)
γ (deg)	82.996(4)	90	90
V (Å^3)	2667.0(8)	5412.7(9)	5484.8(5)
Z	2	4	4
ρ_{calcd} (g/cm^3)	1.548	1.526	1.593
μ (Mo Kα) (mm^{-1})	2.629	2.590	2.571
F (000)	1240	2480	2608
Range of transm factors (deg)	1.281-25.009	1.574-25.010	1.384-25.010
Reflns collected	14991	39619	30351
Unique(R_{int})	9316(0.0550)	9489(0.0602)	9657(0.0500)
$R_1{}^a$, $wR_2{}^b$ [I > 2s(I)]	0.0686, 0.1718	0.0319, 0.0805	0.0307, 0.0621
$R_1{}^a$, $wR_2{}^b$ (all data)	0.1285, 0.2101	0.0421, 0.0860	0.0509, 0.0775
GOF on F^2	1.032	1.046	1.011
CCDC number	1527197	1527198	1527194

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

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

Table S2. The selected bond lengths and angles of **Ir2**, **Ir3** and **Ir4**.

	Ir2	**Ir3**	**Ir4**
Selected bonds	Bond length (Å)	Bond length (Å)	Bond length (Å)
Ir(1)-C(1)	1.978(8)	1.966(4)	1.966(4)
Ir(1)-C(21)	1.998(8)	1.955(4)	1.966(4)
Ir(1)-N(1)	2.054(6)	2.076(3)	2.058(3)
Ir(1)-N(3)	2.045(7)	2.053(3)	2.077(3)
Ir(1)-O(1)	2.231(5)	2.191(3)	2.233(3)
Ir(1)-O(2)	2.277(5)	2.229(3)	2.245(3)
P(1)-O(1)	1.523(5)	1.507(3)	1.515(3)
P(2)-O(2)	1.526(5)	1.513(3)	1.521(3)
P(1)-N(5)	1.592(6)	1.575(4)	1.580(4)
P(2)-N(5)	1.581(6)	1.580(4)	1.583(4)
Selected angles	(°)	(°)	(°)
C(1)-Ir(1)-C(21)	89.9(3)	90.78(16)	90.43(17)
C(1)-Ir(1)-N(1)	97.3(3)	96.88(15)	94.92(16)
C(21)-Ir(1)-N(1)	78.6(3)	79.77(15)	80.02(15)
C(1)-Ir(1)-N(3)	79.8(3)	79.45(15)	79.66(15)
C(21)-Ir(1)-N(3)	95.0(3)	98.95(15)	96.24(15)
C(1)-Ir(1)-O(1)	86.8(2)	86.54(13)	94.53(14)
C(1)-Ir(1)-O(2)	175.6(2)	176.13(12)	174.89(14)
C(21)-Ir(1)-O(1)	175.2(2)	174.87(13)	174.70(14)
C(21)-Ir(1)-O(2)	94.8(2)	95.38(14)	87.22(14)
N(1)-Ir(1)-N(3)	173.0(2)	173.42(13)	173.45(13)
N(1)-Ir(1)-O(2)	81.6(2)	78.34(12)	80.21(12)
N(3)-Ir(1)-O(2)	104.7(2)	105.28(11)	105.10(12)
N(1)-Ir(1)-O(1)	101.0(2)	101.71(13)	101.38(12)
N(3)-Ir(1)-O(1)	82.5(2)	79.99(12)	82.83(12)
O(1)-Ir(1)-O(2)	88.57(17)	87.49(10)	87.98(10)

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

Complex	E_{ox} (V) [a)]	HOMO (eV) [b)]	LUMO (eV)	E_g (eV)
Ir1	0.706	-5.37	-3.56	1.81
Ir2	0.809	-5.48	-3.68	1.80
Ir3	0.870	-5.54	-3.65	1.89
Ir4	0.977	-5.64	-3.75	1.89

[a)] Oxidation potential measured in solution at 0.05 mV/s.

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

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	tpip
Ir1	HOMO	-5.359	2.908	49.15	46.66	4.18
	LUMO	-2.451		4.00	94.41	1.59
Ir2	HOMO	-5.441	2.866	48.12	47.75	4.14
	LUMO	-2.575		3.96	94.42	1.62
Ir3	HOMO	-5.523	3.025	45.83	50.02	4.15
	LUMO	-2.498		3.77	94.67	1.57
Ir4	HOMO	-5.604	2.983	44.29	51.65	4.06
	LUMO	-2.621		3.74	94.67	1.59

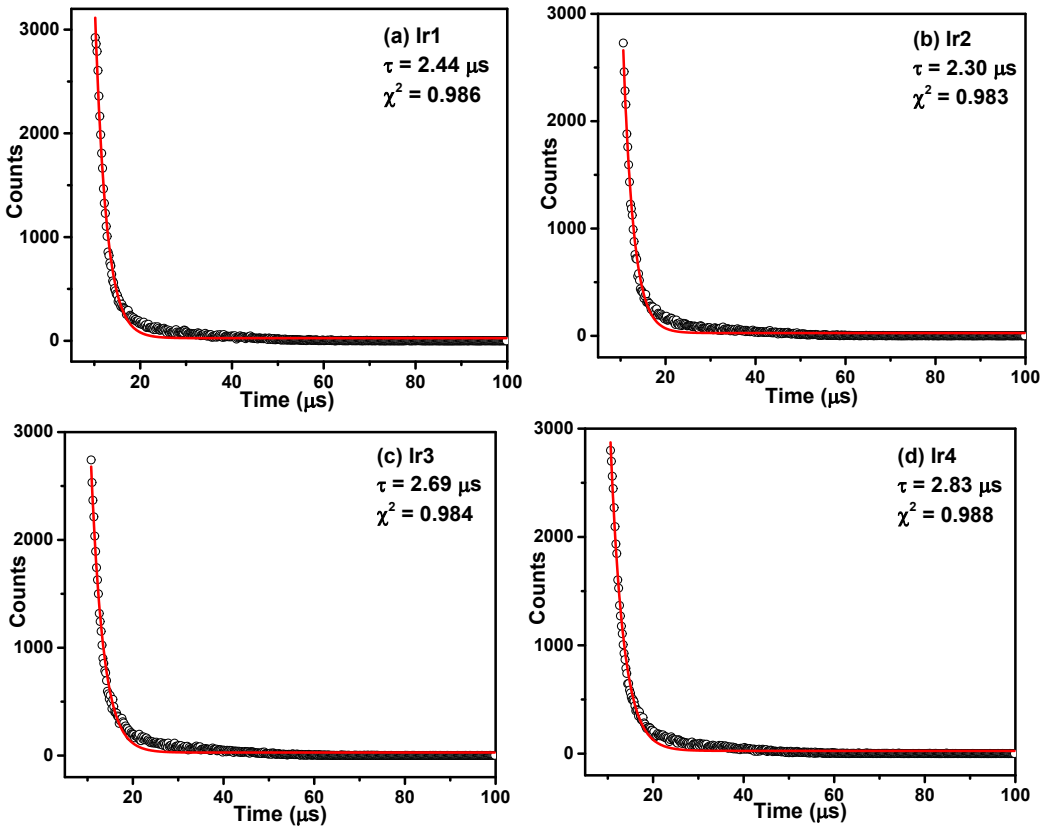

Fig. S1. The lifetime curves of (a) **Ir1**, (b) **Ir2**, (c) **Ir3** and (d) **Ir4** in degassed solution at room temperature.

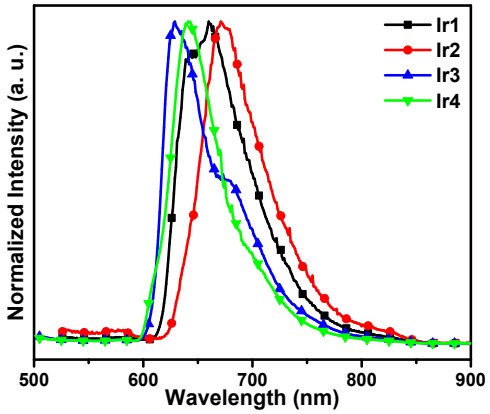

Fig. S2. Normalized PL spectra of **Ir1**, **Ir2**, **Ir3** and **Ir4** in degassed CH_2Cl_2 solutions (5×10^{-5} mol·L^{-1}) at 77 K.

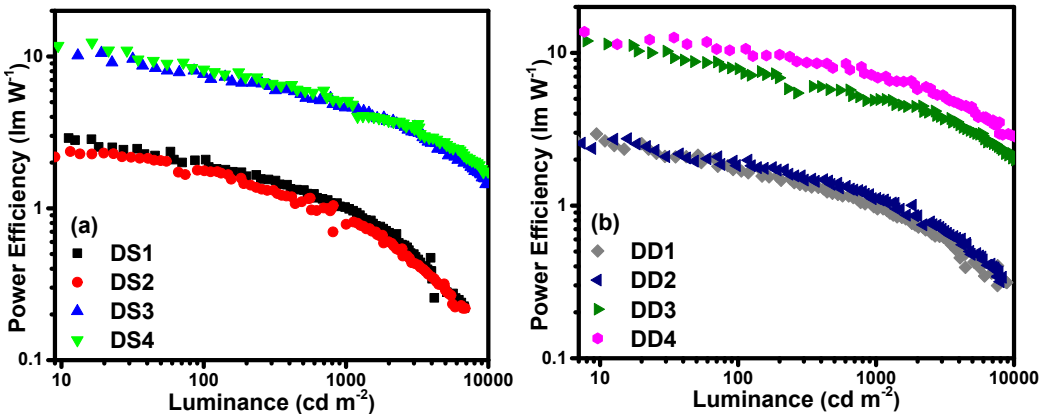

Fig. S3. Power efficiency-luminance (η_p-L) curves of devices (a) **DS1**-**DS4** and (b) **DD1**-**DD4**.