Supporting Information

Efficienct OLEDs with low efficiency roll-off using iridium complexes possessing good electron mobility

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Table S1. Crystallographic data and structure refinement for complexes **L1**, **Ir1** and **Ir2**.

	L1	**Ir1**	**Ir2**
Formula	C_{12} H_6 F_6 N_2	$C_{48}H_{30}F_{12}$ $IrN_5O_2P_2$	$C_{48}H_{30}F_{12}$ $IrN_5O_2P_2$
FW	292.19	1190.93	1190.93
T (K)	296(2)	291(2)	291(2)
Wavelength (Å)	291(2)	0.71073	0.71073
Cryst syst	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/m$	*P-1*	$P2_1/c$
a (Å)	5.0632(16)	15.798(2)	13.6205(10)
b (Å)	15.0923(17)	18.067(2)	23.0074(17)
c (Å)	8.2579(12)	18.657(3)	16.9123(13)
α (deg)	90	83.329(2)	90
β (deg)	104.839(3)	87.048(3)	98.8690(10)
γ (deg)	90	85.597(2)	90
V (Å^3)	610.0(2)	5268.5(12)	5236.5(7)
Z	2	4	4
ρ_{calcd} (g/cm^3)	1.591	1.501	1.511
μ (Mo Kα) (mm^{-1})	0.161	2.678	2.694
F (000)	292	2336	2336
Range of transm factors (deg)	2.55-27.97	1.10-26.00	1.51-25.00
Reflns collected	4090	31907	28777
Unique	1481	20600	9208
GOF on F^2	1.049	1.024	1.116
$R_1{}^a$,$wR_2{}^b$ (I>2σ(I))	0.0468,0.1002	0.0598, 0.1524	0.0545, 0.1615
$R_1{}^a$,$wR_2{}^b$(all data)	0.0711, 0.1019	0.0631, 0.1526	0.0864, 0.1840
CCDC NO.	996478	996479	996480

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

Table S2. The table of selected bond lengths and angles of **L1**, **Ir1** and **Ir2**.

L1					
Selected bonds					
C(1)-C(2)	1.345(2)	C(1)-N(1)	1.355(2)	C(1)-C(8)	1.520(3)
C(2)-C(3)	1.416(2)	C(3)-C(4)	1.443(4)	C(4)-N(2)	1.344(2)
C(4)-C(5)	1.344(2)	C(5)-C(6)	1.341(2)	C(6)-C(7)	1.352(2)
C(8)-F(1)	1.250(5)	C(8)-F(2)	1.265(4)	C(8)-F(1')	1.299(4)
C(8)-F(2')	1.306(5)	C(8)-F(3')	1.345(4)	C(8)-F(3)	1.383(4)
Selected angles					
C(2)-C(1)-N(1)	126.24(18)	C(2)-C(1)-C(8)	120.51(19)	N(1)-C(1)-C(8)	113.21(19)
C(1)-C(2)-C(3)	120.18(18)	C(2)-C(3)-C(4)	122.80(13)	C(5)-C(4)-C(3)	120.76(14)
C(6)-C(5)-C(4)	120.2(2)	C(5)-C(6)-C(7)	122.9(2)	F(1)-C(8)-F(2)	106.2(5)
F(1)-C(8)-F(3)	100.4(3)	F(3)-C(8)-C(1)	107.4(2)	F(2)-C(8)-F(3)	112.2(3)
Ir1					
Selected bonds					
C(1)-C(6)	1.340(16)	C(1)-C(2)	1.405(16)	C(1)-P(1)	1.811(11)
C(2)-C(3)	1.401(19)	C(3)-C(4)	1.35(2)	C(4)-C(5)	1.27(2)
C(5)-C(6)	1.406(17)	C(25)-N(2)	1.326(12)	C(25)-C(26)	1.330(15)
C(26)-C(27)	1.336(17)	C(27)-C(28)	1.403(18)	C(28)-C(29)	1.364(14)
C(29)-N(2)	1.361(12)	C(29)-C(30)	1.479(14)	C(30)-C(34)	1.358(14)
C(30)-C(31)	1.419(13)	C(31)-C(32)	1.429(13)	C(31)-Ir(1)	2.039(9)
C(32)-N(4)	1.307(12)	C(33)-N(4)	1.328(14)	C(33)-C(36)	1.462(19)
C(33)-C(34)	1.346(15)	C(36)-F(6)	1.304(19)	C(36)-F(4)	1.31(2)
C(36)-F(5)	1.33(2)	C(45)-Ir(1)	2.012(9)	Ir(1)-N(3)	2.031(8)
Ir(1)-N(2)	2.061(8)	Ir(1)-O(1)	2.184(6)	Ir(1)-O(2)	2.188(6)
N(1)-P(2)	1.579(8)	N(1)-P(1)	1.600(8)	O(1)-P(1)	1.514(7)
O(2)-P(2)	1.526(7)				
Selected angles					
C(45)-Ir(1)-N(3)	80.5(4)	C(45)-Ir(1)-N(2)	104.2(4)	N(3)-Ir(1)-C(31)	102.7(3)
O(1)-Ir(1)-O(2)	88.5(2)	O(1)-P(1)-C(1)	110.7(5)	O(1)-P(1)-C(7)	107.9(5)
O(1)-P(1)-N(1)	115.9(4)	O(2)-P(2)-N(1)	117.5(4)	O(2)-P(2)-C(19)	106.8(4)
O(2)-P(2)-C(13)	108.9(4)				
Ir2					
Selected bonds					
C(1)-C(2)	1.380(10)	C(1)-C(6)	1.438(9)	C(1)-P(1)	1.771(6)
C(2)-C(3)	1.368(9)	C(2)-C(3)	1.368(9)	C(3)-C(4)	1.397(10)
C(4)-C(5)	1.334(11)	C(5)-C(6)	1.401(10)	C(37)-N(3)	1.353(7)
C(37)-C(38)	1.361(9)	C(38)-C(39)	1.355(10)	C(39)-C(40)	1.389(10)
C(40)-C(41)	1.383(8)	C(41)-N(3)	1.390(6)	C(41)-C(43)	1.465(8)
C(42)-C(43)	1.345(9)	C(42)-N(4)	1.353(7)	C(43)-C(44)	1.385(9)
C(44)-C(45)	1.430(8)	C(45)-C(46)	1.396(10)	C(46)-C(47)	1.506(10)

C(46)-N(4)	1.396(7)	C(47)-F(8)	1.156(8)	C(47)-F(9)	1.264(9)
C(47)-F(7)	1.333(9)	Ir(1)-N(3)	2.004(6)	Ir(1)-N(1)	2.006(5)
Ir(1)-O(1)	2.125(5)	Ir(1)-O(2)	2.167(4)	C(32)-Ir(1)	1.977(6)
C(44)-Ir(1)	1.868(7)	N(5)-P(2)	1.551(6)	N(5)-P(1)	1.591(5)
O(1)-P(1)	1.490(5)	O(2)-P(2)	1.498(5)		
Selected angles					
N(3)-C(41)-C(43)	110.7(5)	C(43)-C(44)-Ir(1)	121.3(5)	C(32)-Ir(1)-N(1)	80.06(19)
C(44)-Ir(1)-N(3)	79.22(17)	O(1)-Ir(1)-O(2)	88.27(18)	P(2)-N(5)-P(1)	124.0(4)
P(1)-O(1)-Ir(1)	126.1(3)	P(2)-O(2)-Ir(1)	125.6(3)	O(1)-P(1)-N(5)	116.7(3)
O(2)-P(2)-N(5)	116.6(3)	O(1)-P(1)-C(1)	107.5(2)	O(1)-P(1)-C(7)	107.6(2)
C(41)-N(3)-Ir(1)	116.5(3)				

Table S3. The orbital distributions of complexes **Ir1**, **Ir2**, **IrA** and **IrB**.

Group		**Ir1**	**IrA**	**Ir2**	**IrB**
Ir (%)	LUMO	3.74	3.34	3.08	3.52
	HOMO	56.39	55.95	54.78	51.73
Main ligand (%)	LUMO	94.25	94.78	94.39	93.50
	HOMO	34.39	37.51	37.55	42.38
tpip (%)	LUMO	2.01	1.88	2.53	2.98
	HOMO	9.22	6.55	7.67	5.89

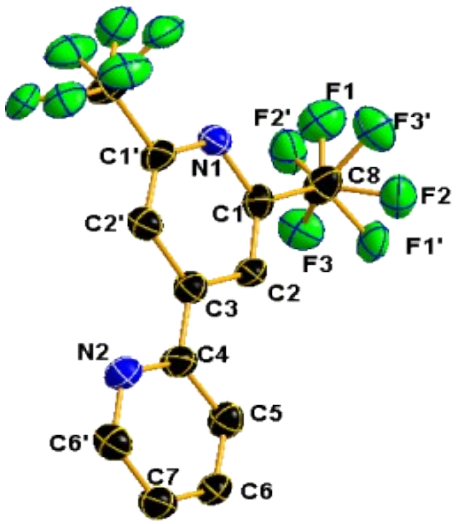

Figure S1. Oak Ridge Thermal Ellipsoidal plot (ORTEP) diagrams of ligand **L2** with the atom-numbering schemes. Hydrogen atoms are omitted for clarity. Ellipsoids are drawn at 30% probability level.

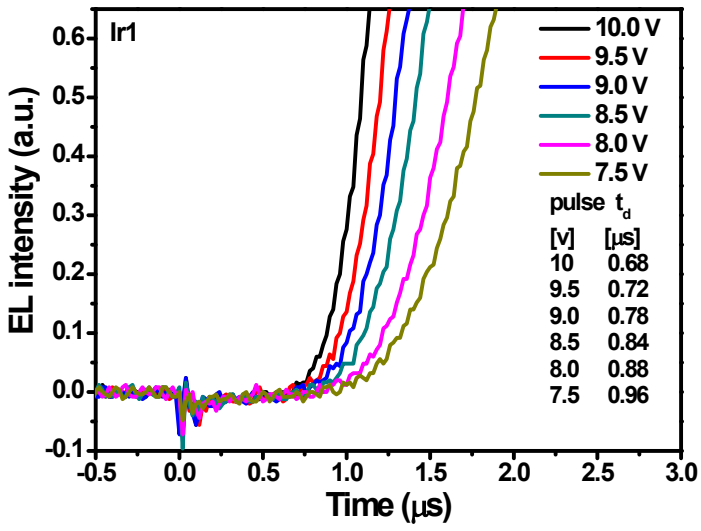

Figure S2. The transient EL signals for the device structure of ITO / TAPC (50 nm) / **Ir1** (60 nm) under different applied fields.

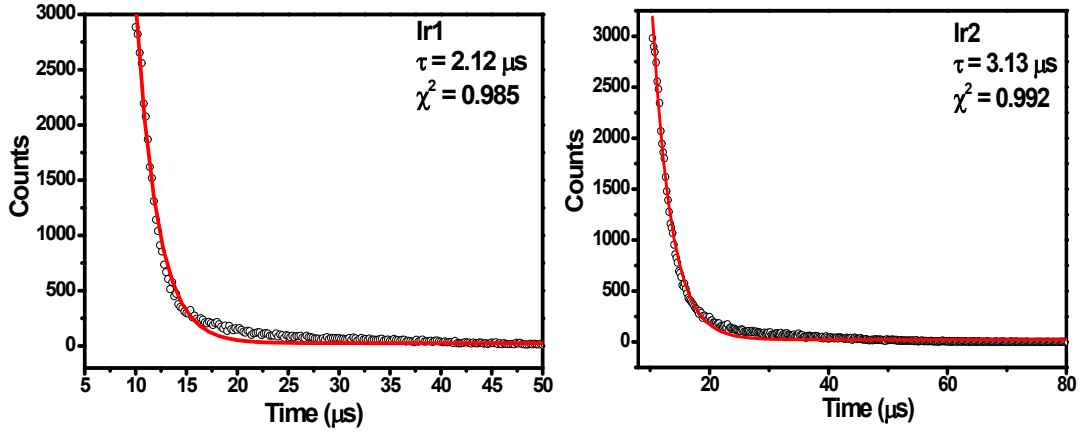

Figure S3. The lifetime curves of **Ir1** and **Ir2** in degassed solution at room temperture.

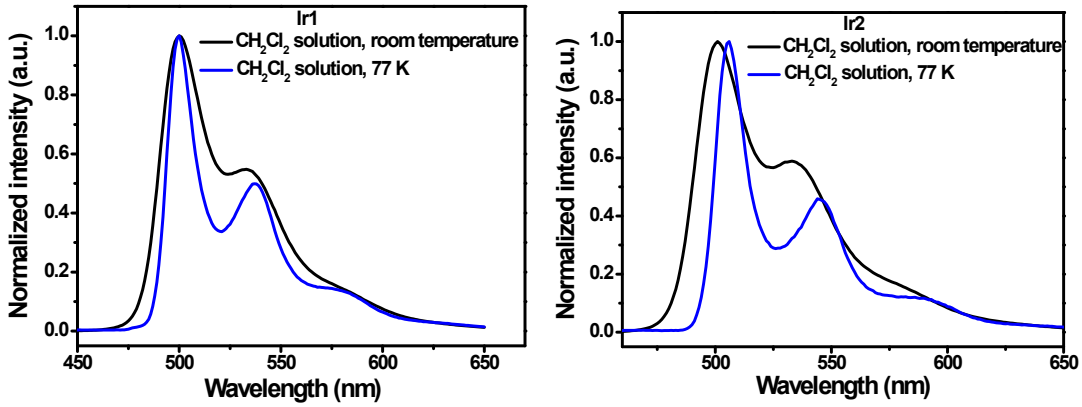

Figure S4. The normalized emission spectra of **Ir1** and **Ir2** in CH_2Cl_2 solution at room temperature and 77 K.

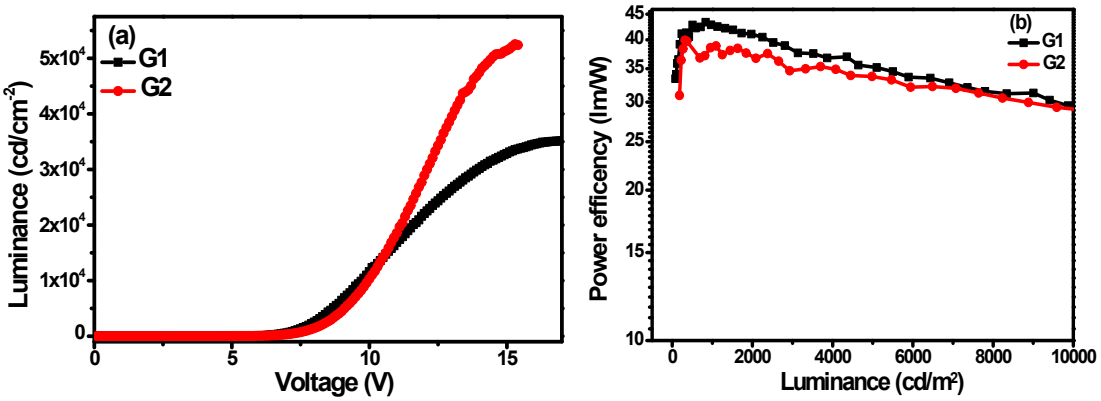

Figure S5. (a) Voltage - luminance (V - L) and (b) power efficiency - luminance (η_p - L) curves of **G1** and **G2** with configuration ITO / TAPC (40 nm) / mCP (10 nm)/ Ir complex (8 wt%): PPO21 (25 nm) / TmPyPB (50 nm) / LiF (1 nm) / Al (100 nm).