Supporting Information

Efficient orange-red electroluminescence of iridium complexes with 1-(2,6-*bis*(trifluoromethyl)pyridin-4-yl)isoquinoline and 4-(2,6-*bis*(trifluoromethyl)pyridin-4-yl)quinazoline ligands

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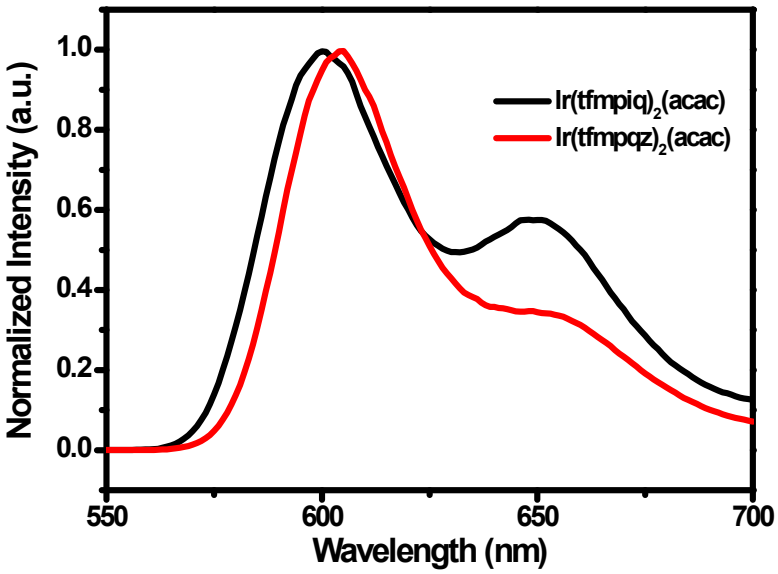

Fig. S1. Emission spectra of $Ir(tfmpiq)_2(acac)$ and $Ir(tfmpqz)_2(acac)$ complexes in degassed CH_2Cl_2 solutions (5.0×10^{-5} mol L^{-1}) at 77 K.

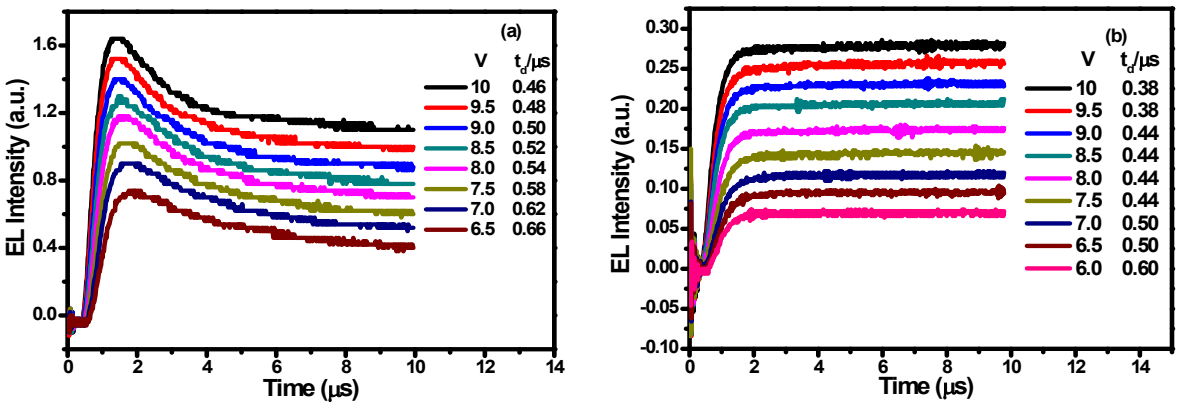

Fig. S2. The transient EL signals for the device structure of ITO/ TAPC (50 nm)/ Ir complexes (60 nm)/ LiF/ Al under different applied fields of $Ir(tfmpiq)_2(acac)$ and $Ir(tfmpqz)_2(acac)$.

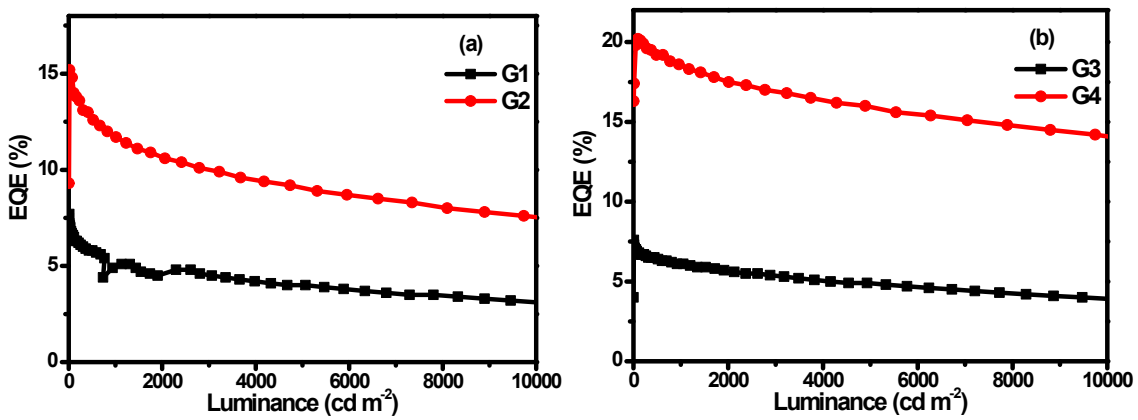

Fig. S3. The external quantum efficiency – luminance (*EQE* – *L*) curves of **G1**, **G2**, **G3** and **G4**.

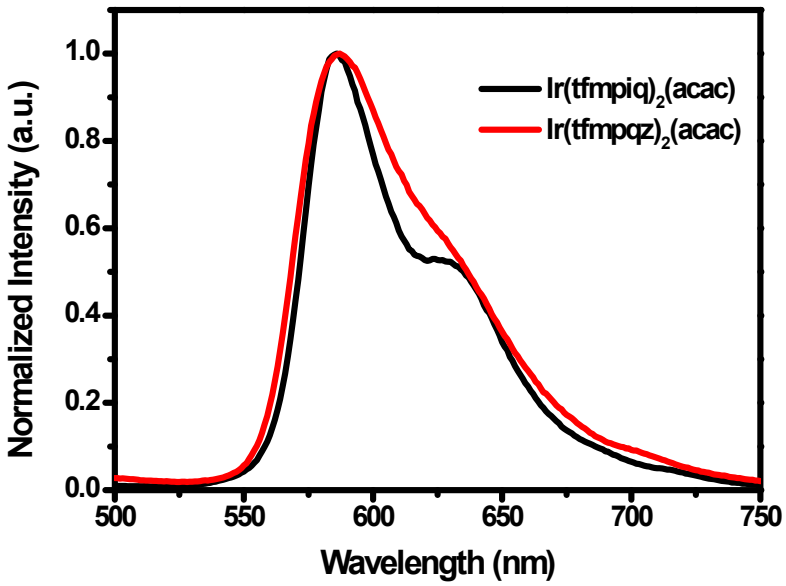

Fig. S4. PL spectra of neat film of the two complexes and light-emitting layers of of $Ir(tfmpiq)_2(acac)$ and $Ir(tfmpqz)_2(acac)$.

Table S1. Crystallographic data of $Ir(tfmpiq)_2(acac)$.

	$Ir(tfmpiq)_2(acac)$
Formula	$C_{37}H_{21}F_{12}IrN_4O_2$
FW	973.97
T (K)	296(2)
Wavelength (Å)	0.71073
Crystal system	triclinic
Space group	*P -1*
a (Å)	11.0271(7)
b (Å)	11.3724(11)
c (Å)	15.8214(19)
α (deg)	83.59
β (deg)	79.73
γ (deg)	71.77
V (Å^3)	1850.9(2)
Z	2
ρ_{calcd} (mg/cm^3)	1.748
μ (Mo Kα) (mm^{-1})	3.706
F (000)	944
Reflns collected	13306
Unique	9053
Data/restraints/params	9053 / 74 / 507
GOF on F^2	0.990
$R_1{}^a$, $wR_2{}^b$ [$I > 2\sigma(I)$]	0.0411, 0.1035
$R_1{}^a$, $wR_2{}^b$ (all data)	0.0561, 0.1112
CCDC NO	1558320

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

Table S2 The selected bond lengths and angels of $Ir(tfmpiq)_2(acac)$.

Selected bonds Å					
Ir(01)-C(00A)	2.012(5)	C(00H)-C(013)	1.506(9)	C(00Y)-H(00Y)	0.93
Ir(01)-C(00B)	2.026(5)	C(00I)-C(00U)	1.381(8)	C(00Z)-C(01I)	1.500(10)
Ir(01)-N(006)	2.049(5)	F(00J)-C(01C)	1.338(11)	F(010)-C(01I)	1.224(12)
Ir(01)-N(004)	2.051(5)	C(00K)-C(014)	1.380(9)	C(011)-H(011)	0.93
Ir(01)-O(002)	2.105(4)	C(00K)-C(012)	1.507(8)	C(012)-H(01A)	0.96
Ir(01)-O(003)	2.113(4)	C(00L)-C(017)	1.384(9)	C(012)-H(01B)	0.96
O(002)-C(00K)	1.269(7)	C(00L)-C(00O)	1.458(8)	C(012)-H(01C)	0.96
O(003)-C(01A)	1.271(7)	C(00M)-C(00R)	1.346(8)	C(014)-C(01A)	1.412(9)
N(004)-C(00O)	1.345(7)	C(00M)-H(00M)	0.93	C(014)-H(014)	0.93
N(004)-C(00T)	1.363(8)	C(00N)-C(00X)	1.356(9)	C(015)-C(01E)	1.408(10)
F(005)-C(013)	1.327(8)	C(00N)-C(00Q)	1.394(10)	C(015)-C(016)	1.411(9)
N(006)-C(00C)	1.340(7)	C(00N)-H(00N)	0.93	C(016)-H(016)	0.93
N(006)-C(00M)	1.359(7)	C(00O)-C(00S)	1.426(8)	C(017)-C(019)	1.381(9)
F(007)-C(013)	1.324(9)	C(00P)-C(00R)	1.402(8)	C(017)-H(017)	0.93
F(008)-C(013)	1.339(7)	C(00P)-C(011)	1.427(8)	F(018)-C(01J)	1.185(15)
F(009)-C(01C)	1.318(8)	C(00Q)-C(011)	1.357(9)	C(019)-C(01J)	1.517(13)
C(00A)-C(00H)	1.423(8)	C(00Q)-H(00Q)	0.93	C(01A)-C(01G)	1.508(9)
C(00A)-C(00L)	1.424(8)	C(00R)-H(00R)	0.93	C(01B)-C(01F)	1.411(11)
C(00B)-C(00V)	1.414(8)	C(00S)-C(015)	1.423(8)	C(01B)-H(01D)	0.93
C(00B)-C(00I)	1.414(8)	C(00S)-C(00Y)	1.427(8)	F(01D)-C(01I)	1.210(16)
C(00C)-C(00G)	1.413(8)	C(00T)-C(016)	1.335(9)	C(01E)-C(01F)	1.355(11)
C(00C)-C(00I)	1.489(8)	C(00T)-H(00T)	0.93	C(01E)-H(01E)	0.93
F(00D)-C(01C)	1.306(10)	C(00U)-C(00Z)	1.392(9)	C(01F)-H(01F)	0.93
N(00E)-C(019)	1.323(10)	C(00U)-H(00U)	0.93	C(01G)-H(01G)	0.96
N(00E)-C(00H)	1.337(8)	C(00V)-C(01C)	1.520(10)	C(01G)-H(01H)	0.96
N(00F)-C(00Z)	1.326(9)	F(00W)-C(01J)	1.299(12)	C(01G)-H(01I)	0.96
N(00F)-C(00V)	1.328(8)	C(00X)-H(00X)	0.93	F(01H)-C(01J)	1.456(18)
C(00G)-C(00P)	1.422(8)	C(00Y)-C(01B)	1.369(10)	C(01I)-F(01K)	1.233(16)
C(00G)-C(00X)	1.429(8)				
Selected angels°					
C(00A)-Ir(01)-C(00B)	93.2(2)	C(00X)-C(00N)-C(00Q)	120.7(6)	C(00K)-C(014)-C(01A)	128.5(6)
C(00A)-Ir(01)-N(006)	106.6(2)	C(00X)-C(00N)-H(00N)	119.6	C(00K)-C(014)-H(014)	115.7
C(00B)-Ir(01)-N(006)	80.1(2)	C(00Q)-C(00N)-H(00N)	119.6	C(01A)-C(014)-H(014)	115.7
C(00A)-Ir(01)-N(004)	80.1(2)	N(004)-C(00O)-C(00S)	120.2(5)	C(01E)-C(015)-C(016)	122.6(6)
C(00B)-Ir(01)-N(004)	106.4(2)	N(004)-C(00O)-C(00L)	111.6(5)	C(01E)-C(015)-C(00S)	120.2(7)
N(006)-Ir(01)-N(004)	170.68(18)	C(00S)-C(00O)-C(00L)	128.2(5)	C(016)-C(015)-C(00S)	117.2(6)
C(00A)-Ir(01)-O(002)	88.28(19)	C(00R)-C(00P)-C(00G)	119.0(5)	C(00T)-C(016)-C(015)	121.0(6)
C(00B)-Ir(01)-O(002)	172.63(18)	C(00R)-C(00P)-C(011)	122.1(6)	C(00T)-C(016)-H(016)	119.5
N(006)-Ir(01)-O(002)	92.59(17)	C(00G)-C(00P)-C(011)	118.9(5)	C(015)-C(016)-H(016)	119.5
N(004)-Ir(01)-O(002)	80.98(17)	C(011)-C(00Q)-C(00N)	120.6(6)	C(019)-C(017)-C(00L)	118.7(6)
C(00A)-Ir(01)-O(003)	172.51(18)	C(011)-C(00Q)-H(00Q)	119.7	C(019)-C(017)-H(017)	120.6
C(00B)-Ir(01)-O(003)	89.45(19)	C(00N)-C(00Q)-H(00Q)	119.7	C(00L)-C(017)-H(017)	120.6
N(006)-Ir(01)-O(003)	80.78(18)	C(00M)-C(00R)-C(00P)	119.7(5)	N(00E)-C(019)-C(017)	123.6(7)
N(004)-Ir(01)-O(003)	92.42(18)	C(00M)-C(00R)-H(00R)	120.2	N(00E)-C(019)-C(01J)	114.9(7)
O(002)-Ir(01)-O(003)	89.97(16)	C(00P)-C(00R)-H(00R)	120.2	C(017)-C(019)-C(01J)	121.4(7)
C(00K)-O(002)-Ir(01)	124.6(4)	C(015)-C(00S)-C(00O)	118.5(5)	O(003)-C(01A)-C(014)	126.0(6)
C(01A)-O(003)-Ir(01)	124.2(4)	C(015)-C(00S)-C(00Y)	116.9(6)	O(003)-C(01A)-C(01G)	114.4(6)
C(00O)-N(004)-C(00T)	120.3(5)	C(00O)-C(00S)-C(00Y)	124.5(5)	C(014)-C(01A)-C(01G)	119.6(6)

C(00O)-N(004)-Ir(01)	115.7(4)	C(016)-C(00T)-N(004)	122.1(6)	C(00Y)-C(01B)-C(01F)	119.5(7)
C(00T)-N(004)-Ir(01)	122.2(4)	C(016)-C(00T)-H(00T)	118.9	C(00Y)-C(01B)-H(01D)	120.3
C(00C)-N(006)-C(00M)	120.2(5)	N(004)-C(00T)-H(00T)	118.9	C(01F)-C(01B)-H(01D)	120.3
C(00C)-N(006)-Ir(01)	116.2(4)	C(00I)-C(00U)-C(00Z)	117.8(6)	F(00D)-C(01C)-F(009)	107.4(7)
C(00M)-N(006)-Ir(01)	121.9(4)	C(00I)-C(00U)-H(00U)	121.1	F(00D)-C(01C)-F(00J)	105.9(7)
C(00H)-C(00A)-C(00L)	113.1(5)	C(00Z)-C(00U)-H(00U)	121.1	F(009)-C(01C)-F(00J)	106.4(7)
C(00H)-C(00A)-Ir(01)	134.4(4)	N(00F)-C(00V)-C(00B)	126.9(6)	F(00D)-C(01C)-C(00V)	113.2(7)
C(00L)-C(00A)-Ir(01)	112.4(4)	N(00F)-C(00V)-C(01C)	110.9(6)	F(009)-C(01C)-C(00V)	112.5(6)
C(00V)-C(00B)-C(00I)	112.6(5)	C(00B)-C(00V)-C(01C)	122.1(6)	F(00J)-C(01C)-C(00V)	111.0(7)
C(00V)-C(00B)-Ir(01)	134.6(4)	C(00N)-C(00X)-C(00G)	121.2(6)	C(01F)-C(01E)-C(015)	120.6(7)
C(00I)-C(00B)-Ir(01)	112.7(4)	C(00N)-C(00X)-H(00X)	119.4	C(01F)-C(01E)-H(01E)	119.7
N(006)-C(00C)-C(00G)	121.0(5)	C(00G)-C(00X)-H(00X)	119.4	C(015)-C(01E)-H(01E)	119.7
N(006)-C(00C)-C(00I)	111.1(5)	C(01B)-C(00Y)-C(00S)	121.7(6)	C(01E)-C(01F)-C(01B)	120.7(7)
C(00G)-C(00C)-C(00I)	127.9(5)	C(01B)-C(00Y)-H(00Y)	119.1	C(01E)-C(01F)-H(01F)	119.6
C(019)-N(00E)-C(00H)	117.2(6)	C(00S)-C(00Y)-H(00Y)	119.1	C(01B)-C(01F)-H(01F)	119.6
C(00Z)-N(00F)-C(00V)	116.9(6)	N(00F)-C(00Z)-C(00U)	123.4(6)	C(01A)-C(01G)-H(01G)	109.5
C(00C)-C(00G)-C(00P)	117.4(5)	N(00F)-C(00Z)-C(01I)	116.8(7)	C(01A)-C(01G)-H(01H)	109.5
C(00C)-C(00G)-C(00X)	124.7(5)	C(00U)-C(00Z)-C(01I)	119.9(7)	H(01G)-C(01G)-H(01H)	109.5
C(00P)-C(00G)-C(00X)	117.8(5)	C(00Q)-C(011)-C(00P)	120.7(6)	C(01A)-C(01G)-H(01I)	109.5
N(00E)-C(00H)-C(00A)	125.9(6)	C(00Q)-C(011)-H(011)	119.7	H(01G)-C(01G)-H(01I)	109.5
N(00E)-C(00H)-C(013)	111.8(5)	C(00P)-C(011)-H(011)	119.7	H(01H)-C(01G)-H(01I)	109.5
C(00A)-C(00H)-C(013)	122.2(5)	C(00K)-C(012)-H(01A)	109.5	F(01D)-C(01I)-F(010)	108.0(12)
C(00U)-C(00I)-C(00B)	121.8(5)	C(00K)-C(012)-H(01B)	109.5	F(01D)-C(01I)-F(01K)	93.3(11)
C(00U)-C(00I)-C(00C)	121.7(5)	H(01A)-C(012)-H(01B)	109.5	F(010)-C(01I)-F(01K)	106.2(14)
C(00B)-C(00I)-C(00C)	116.1(5)	C(00K)-C(012)-H(01C)	109.5	F(01D)-C(01I)-C(00Z)	113.7(13)
O(002)-C(00K)-C(014)	126.6(5)	H(01A)-C(012)-H(01C)	109.5	F(010)-C(01I)-C(00Z)	117.4(8)
O(002)-C(00K)-C(012)	113.7(6)	H(01B)-C(012)-H(01C)	109.5	F(01K)-C(01I)-C(00Z)	115.3(11)
C(014)-C(00K)-C(012)	119.7(6)	F(007)-C(013)-F(005)	106.9(6)	F(018)-C(01J)-F(00W)	115.9(12)
C(017)-C(00L)-C(00A)	120.7(5)	F(007)-C(013)-F(008)	107.4(6)	F(018)-C(01J)-F(01H)	100.4(10)
C(017)-C(00L)-C(00O)	122.2(5)	F(005)-C(013)-F(008)	104.6(6)	F(00W)-C(01J)-F(01H)	99.9(13)
C(00A)-C(00L)-C(00O)	116.6(5)	F(007)-C(013)-C(00H)	111.6(6)	F(018)-C(01J)-C(019)	116.4(13)
C(00R)-C(00M)-N(006)	122.2(5)	F(005)-C(013)-C(00H)	113.6(6)	F(00W)-C(01J)-C(019)	114.3(8)
C(00R)-C(00M)-H(00M)	118.9	F(008)-C(013)-C(00H)	112.3(6)	F(01H)-C(01J)-C(019)	106.8(11)
N(006)-C(00M)-H(00M)	118.9				