

Supporting Information

Two blue iridium complexes for efficient electroluminescence with low efficiency roll-off

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Table S1 Crystallographic data and structure refinement for complexes (dfppy)₂Ir(tpip) and (dfppy)₂Ir(Ftpip)

	(dfppy) ₂ Ir(tpip)	(dfppy) ₂ Ir(Ftpip)
Formula	C ₄₄ H ₃₀ F ₄	C ₄₄ H ₂₆ F ₈
	IrN ₅ O ₂ P ₂	IrN ₅ O ₂ P ₂
FW	990.90	1062.84
T (K)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> (Å)	11.523 (3)	20.944(5)
<i>b</i> (Å)	16.473 (2)	19.770(5)
<i>c</i> (Å)	20.708 (3)	21.011(5)
<i>α</i> (deg)	90.00	90.00
<i>β</i> (deg)	90.00	106.420(4)
<i>γ</i> (deg)	90.00	90.00
<i>V</i> (Å³)	3930.8(15)	8345(4)
<i>Z</i>	4	8
<i>ρ</i>_{calcd} (mg/cm³)	1.674	1.692
<i>μ</i> (Mo Kα) (mm⁻¹)	3.543	3.357
<i>F</i> (000)	1952	4160
Reflns collected	23539	71484
Unique	7729	18321
Data/restraints/params	7729 / 0 / 523	18321 / 0 / 1117
GOF on <i>F</i>²	0.892	0.991
<i>R</i>₁^{<i>a</i>}, <i>wR</i>₂^{<i>b</i>} [<i>I</i> > 2σ(<i>I</i>)]	0.0292, 0.0630	0.0357, 0.0885
<i>R</i>₁^{<i>a</i>}, <i>wR</i>₂^{<i>b</i>} (all data)	0.0380, 0.0648	0.0628, 0.1007
CCDC NO	1062396	1062397

$$R_1^a = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad wR_2^b = \left[\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)} \right]^{1/2}$$

Table S2 The table of selected bond lengths of (dfppy)₂Ir(tpip) and (dfppy)₂Ir(Ftpip)

(dfppy) ₂ Ir(tpip)					
Selected bonds					
Ir(1)-C(1)	1.982(4)	Ir(1)-O(1)	2.202(2)	Ir(1)-N(4)	2.048(3)
Ir(1)-C(11)	1.970(3)	Ir(1)-O(2)	2.177(2)	Ir(1)-N(5)	2.044(3)
O(2)-P(2)	1.521(3)	N(1)-P(2)	1.591(3)	C(4)-N(2)	1.302(6)
O(1)-P(1)	1.522(2)	N(1)-P(1)	1.590(3)	C(3)-N(2)	1.303(6)
C(3)-F(1)	1.352(5)	C(4)-F(2)	1.355(5)		
(dfppy) ₂ Ir(Ftpip)					
Selected bonds					
Ir(2)-C(45)	1.971(5)	Ir(2)-O(4)	2.180(3)	Ir(2)-N(8)	2.034(4)
Ir(2)-C(55)	1.965(5)	Ir(2)-O(3)	2.176(3)	Ir(2)-N(9)	2.030(4)
O(3)-P(9)	1.511(3)	N(10)-P(9)	1.587(4)	C(43)-N(6)	1.288(8)
O(4)-P(11)	1.504(3)	N(10)-P(11)	1.579(4)	C(47)-N(6)	1.290(8)
C(43)-F(13)	1.352(7)	C(47)-F(14)	1.355(7)		

Table S3. The orbital distributions of complexes (dfppy)₂Ir(tpip) and (dfppy)₂Ir(Ftpip).

Group		(dfppy) ₂ Ir(tpip)	(dfppy) ₂ Ir(Ftpip)
Ir (%)	LUMO	5.02	5.02
	HOMO	56.22	56.11
dfppy (%)	LUMO	91.53	90.97
	HOMO	37.36	35.36
tpip /Ftpip (%)	LUMO	3.45	4.01
	HOMO	6.41	8.52

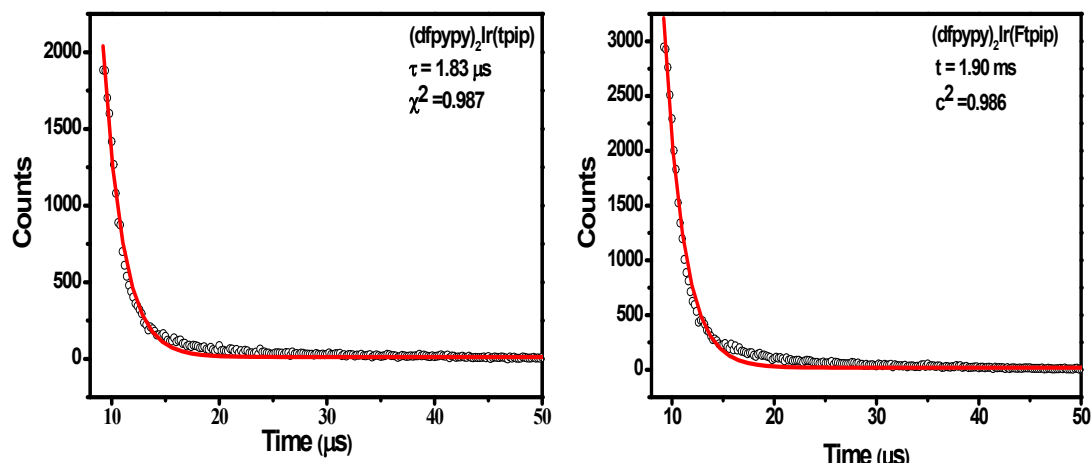


Figure S1. The lifetime curves of $(dfppy)_2Ir(tpip)$ and $(dfppy)_2Ir(Ftpip)$ in degassed CH_2Cl_2 solution at room temperature.

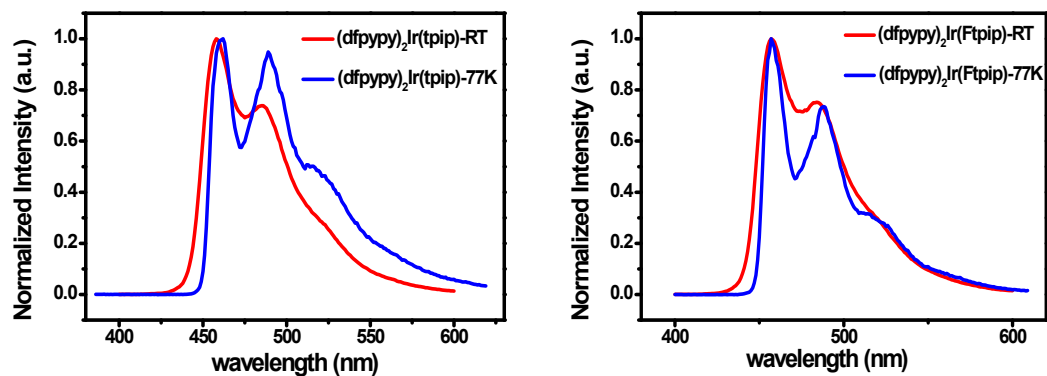


Figure S2. The normalized emission spectra of $(dfppy)_2Ir(tpip)$ and $(dfppy)_2Ir(Ftpip)$ in CH_2Cl_2 solution at room temperature and 77 K.

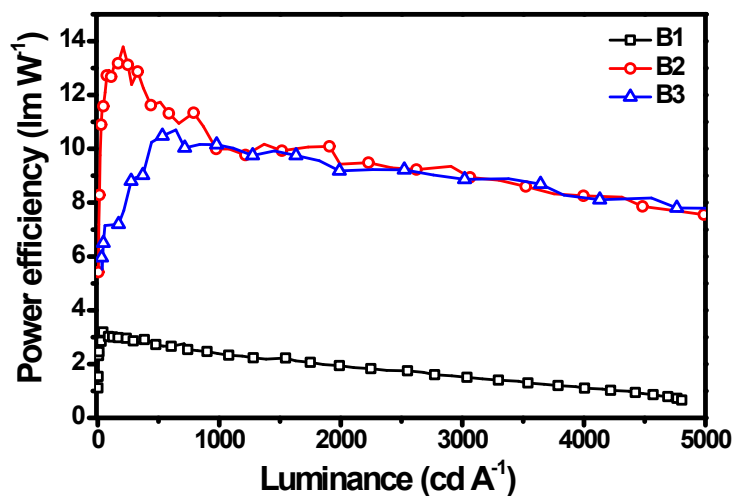


Figure S3. The power efficiency–luminance (η_p – L) curves of device **B1**, **B2** and **B3**.