Electronic Supplementary Information

for

Novel iridium(III) complexes bearing dimesityboron group with nearly 100% phosphorescent quantum yields for highly efficient organic light-emitting diodes†

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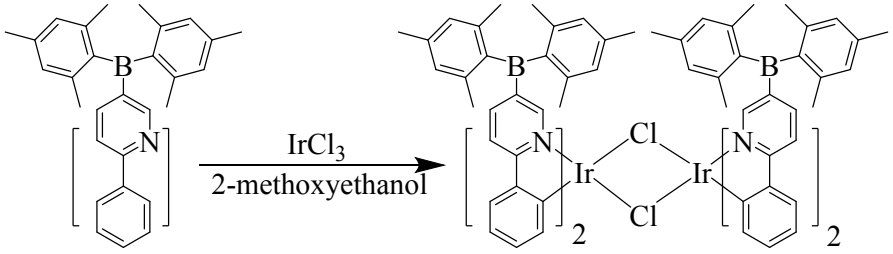
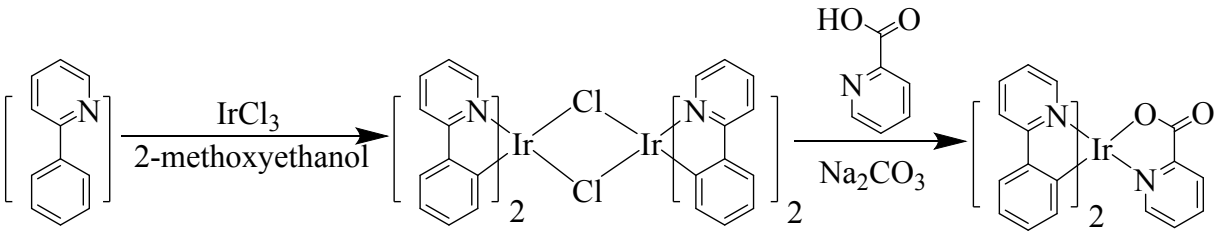
Scheme S1 Synthetic pathway for the Ir(III)-μ-chloride-bridged dimer **Ir[ppyB]$_2$Cl$_2$**.



HppyB **Ir[ppyB]$_2$Cl$_2$**

Both **HppyB** and **Ir[ppyB]$_2$Cl$_2$** were synthesized following our previously reported methods.[1]

Scheme S2 Synthetic pathway for the parent complex **Ir[ppy]$_2$[pic]**.



Hppy **Ir[ppy]$_2$Cl$_2$** **Ir[ppy]$_2$[pic]**

Both **Ir[ppy]$_2$Cl$_2$** and **Ir[ppy]$_2$[pic]** were synthesized following the literature methods.[2]

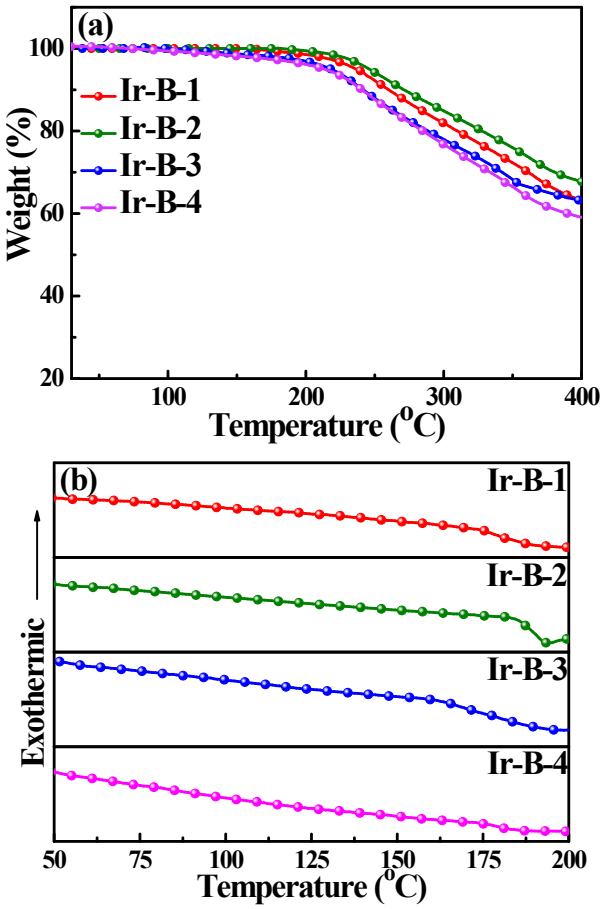


Fig. S1 (a) TGA and (b) DSC curves for the cyclometalated iridium(III) complexes.

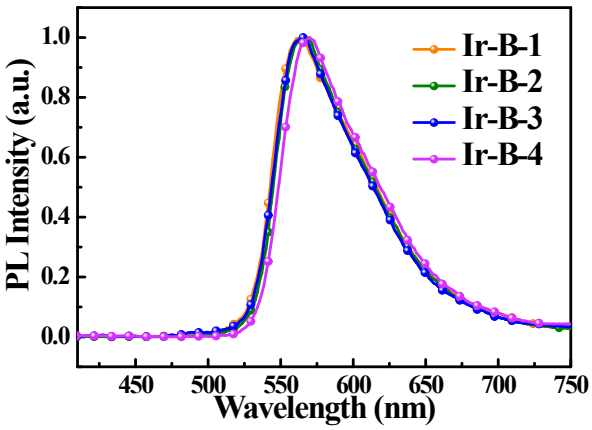


Fig. S2 PL spectra for the phosphorescent complexes in CH_2Cl_2 with 10^{-5} M at 77 K.

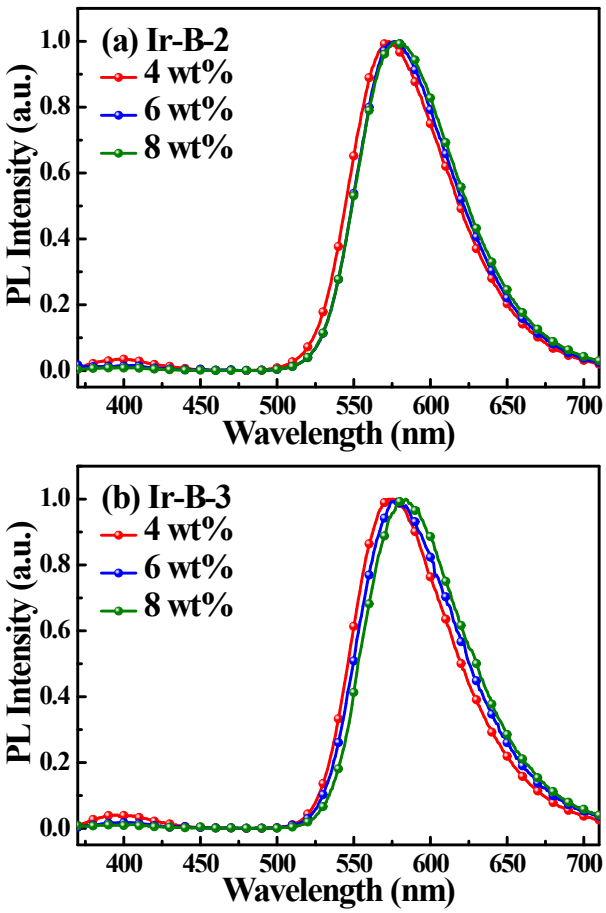


Fig. S3 PL spectra for (a) **Ir-B-2** and (b) **Ir-B-3** doped in TCTA film at 298 K.

Table S1 PL data for **Ir-B-2** and **Ir-B-3** doped in TCTA film at 298 K.

Compound	Doping level	Emission λ_{em} (nm)	Absolute Φ_p (%) [a]
Ir-B-2	4 wt%	396, 573	99
	6 wt%	577	100
	8 wt%	580	100
Ir-B-3	4 wt%	396, 574	100
	6 wt%	578	100
	8 wt%	582	100

[a] Measured in an integrating sphere with doped TCTA film on quartz as sample and the excitation wavelength was set at 360 nm. The data were obtained by the average for the three-time measurement.

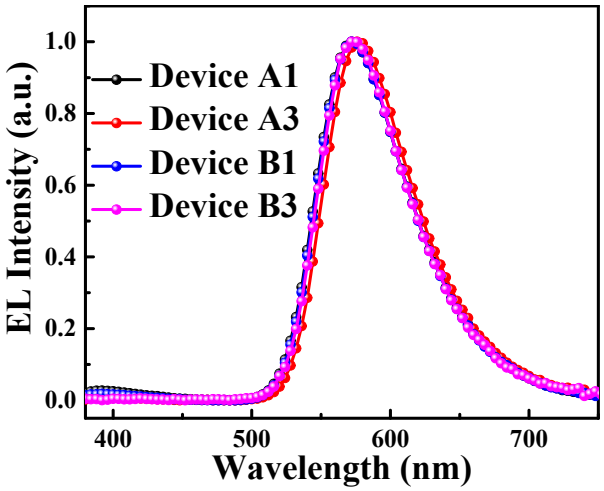
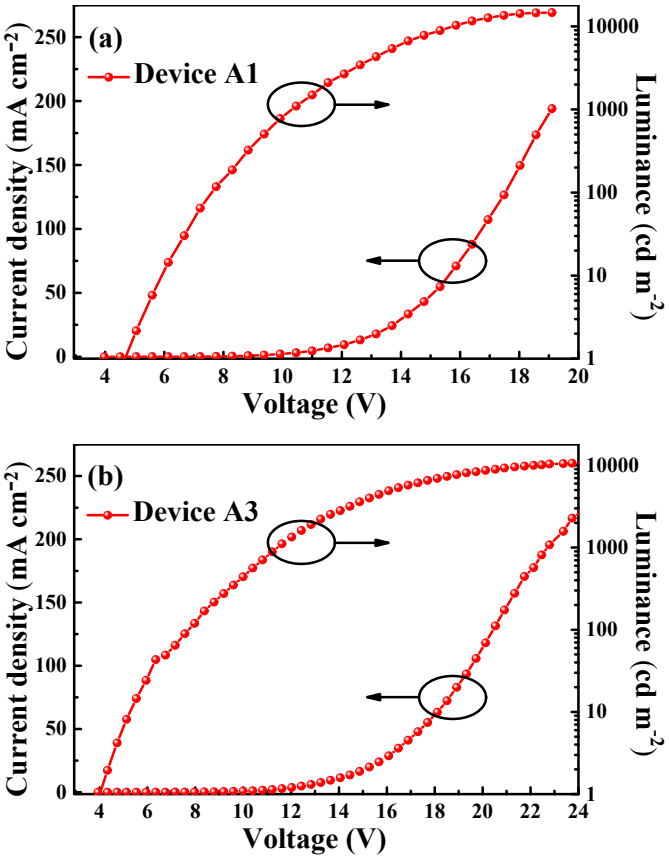


Fig. S4 EL spectra for devices **A1**, **A3**, **B1**, and **B3** at *ca.* 10 V.



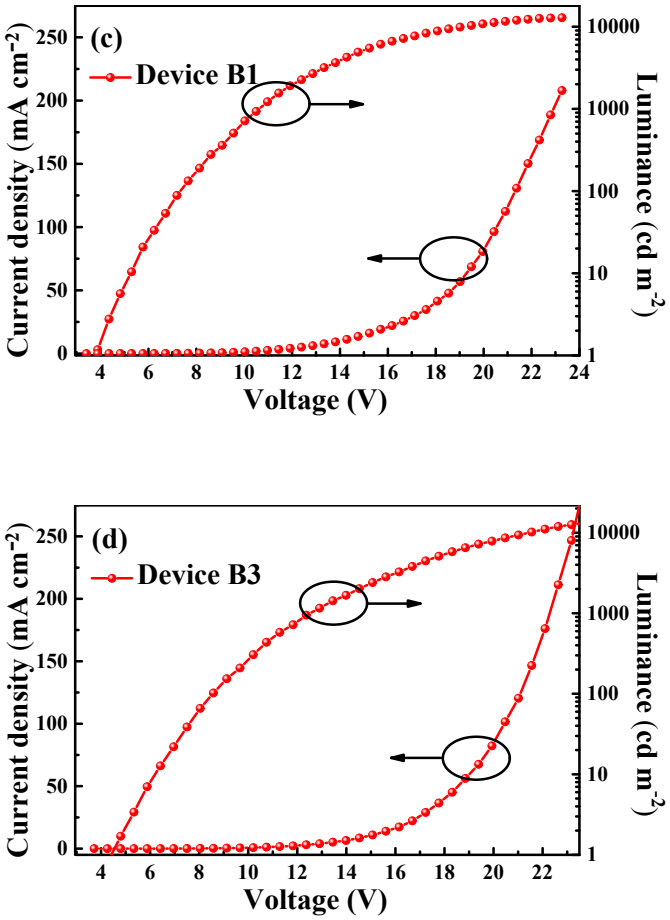
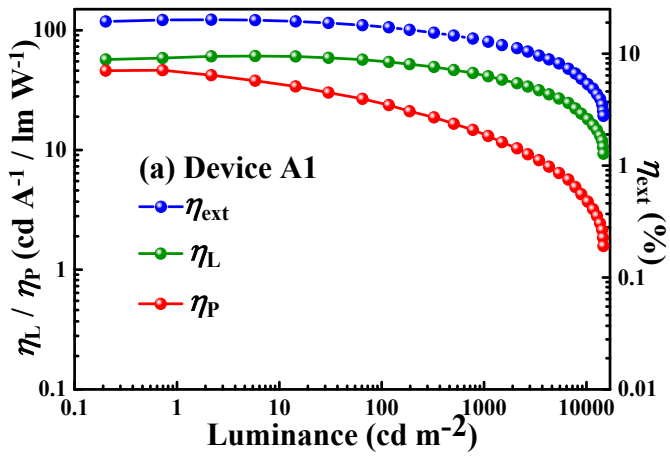


Fig. S5 Current density (*J*)–voltage (*V*)–luminance (*L*) curves for the devices (a) **A1**, (b) **A3**, (c) **B1** and (d) **B3.**



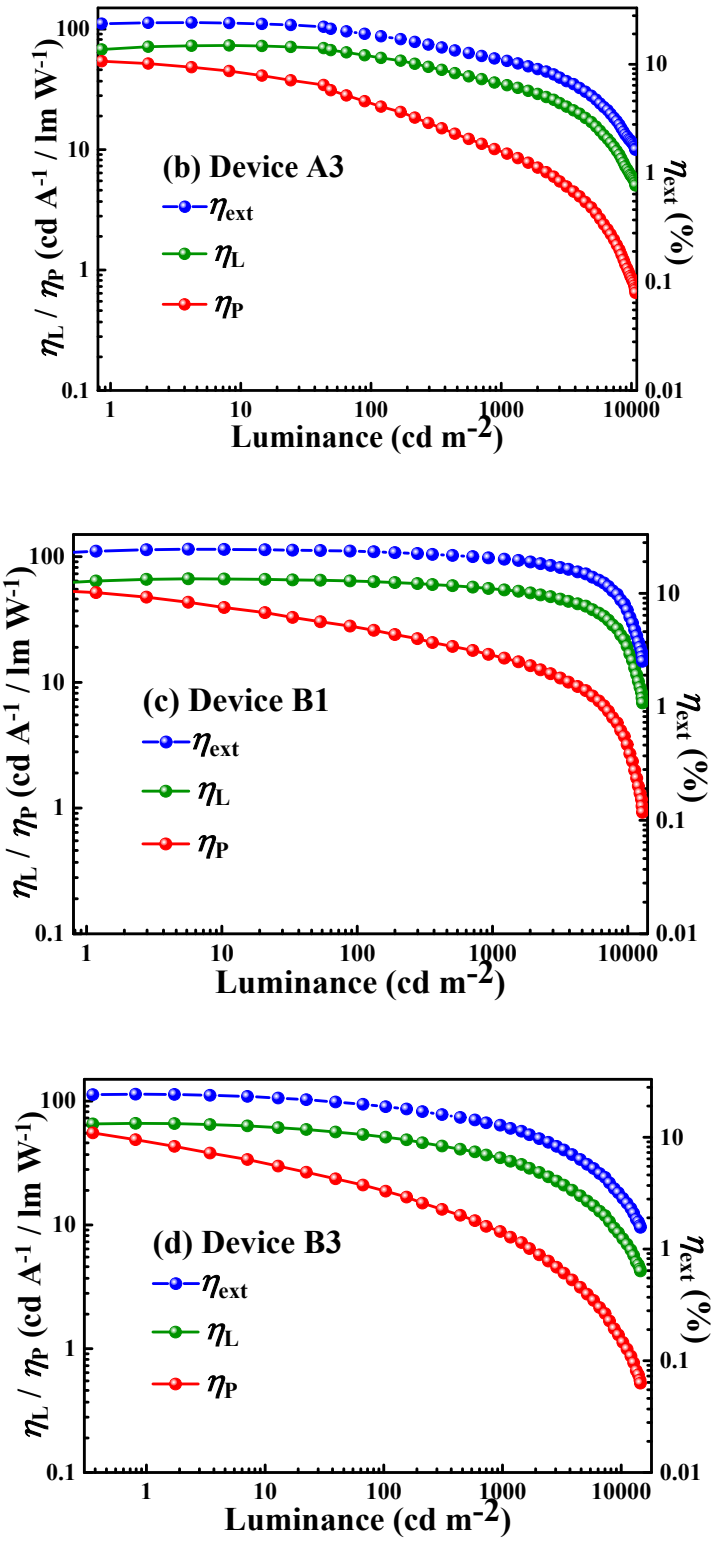


Fig. S6 Relationship between EL efficiencies and current density for the devices (a) **A1**, (b) **A3**, (c) **B1** and (d) **B3**.

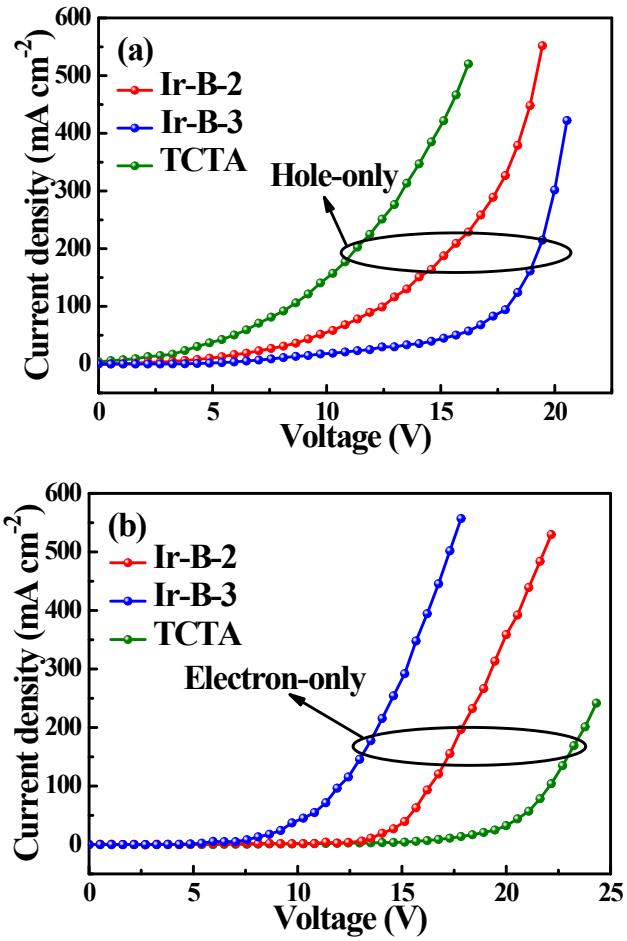


Fig. S3 Current density-voltage (*J-V*) curves for (a) hole-only devices and (b) electron-only devices of neat film for **Ir-B-2**, **Ir-B-3** and **TCTA**. Hole-only device: ITO/MoO_3 (3 nm)/PEDOT: PSS (20 nm)/active layer (50 nm)/NPB (30 nm)/MoO_3 (3 nm)/Al (100 nm). Electron-only device: ITO/LiF (3 nm)/active layer (50 nm)/LiF (3 nm)/Al (100 nm).

References

1 X. Yang, N. Sun, J. Dang, Z. Huang, C. Yao, X. Xu, C. L. Ho, G. Zhou, D. Ma, X. Zhao and W. Y. Wong, *J. Mater. Chem. C*, 2013, **1**, 3317.

2 H. Sun, L. Yang, H. Yang, S. Liu, W. Xu, X. Liu, Z. Tu, H. Su, Q. Zhao and W. Huang, *RSC Adv.*, 2013, **3**, 8766.