

## Electronic Supplementary Material

# **Ir<sup>III</sup>(C<sup>^</sup>N)<sub>2</sub>(P-donor ligand)Cl-type complexes bearing functional groups and showing aggregation-induced phosphorescent emission (AIPE) behavior for highly efficient OLEDs**

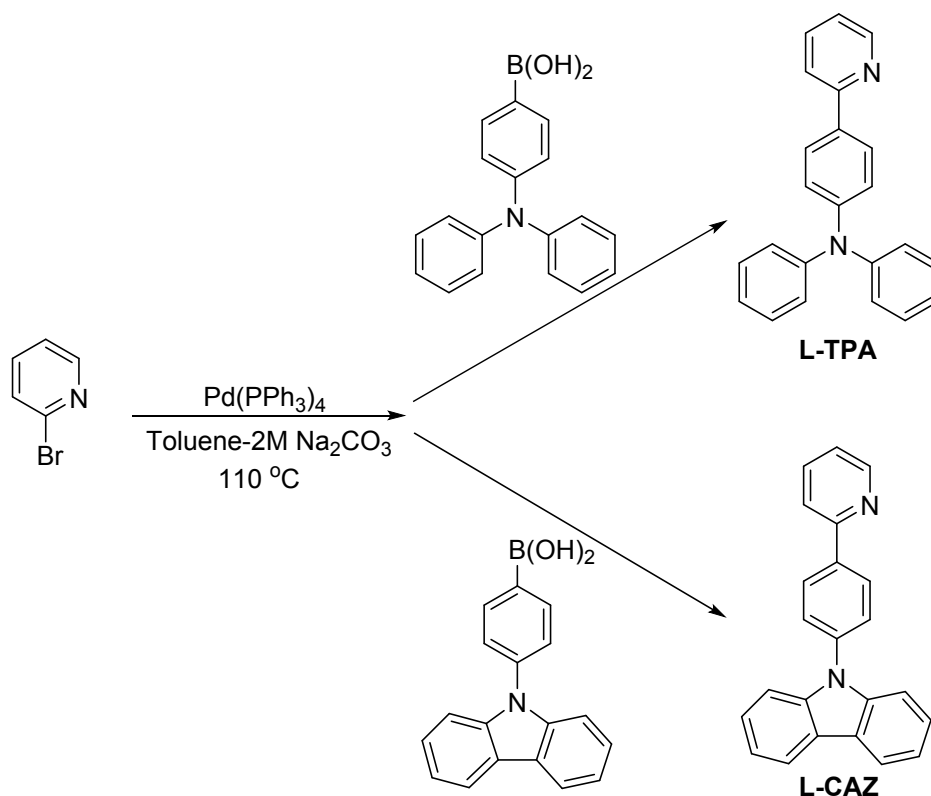
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**Scheme S1.** Synthetic scheme for the C<sup>N</sup>-type ligands.

### Procedures for the synthesis of C<sup>N</sup>-type ligands

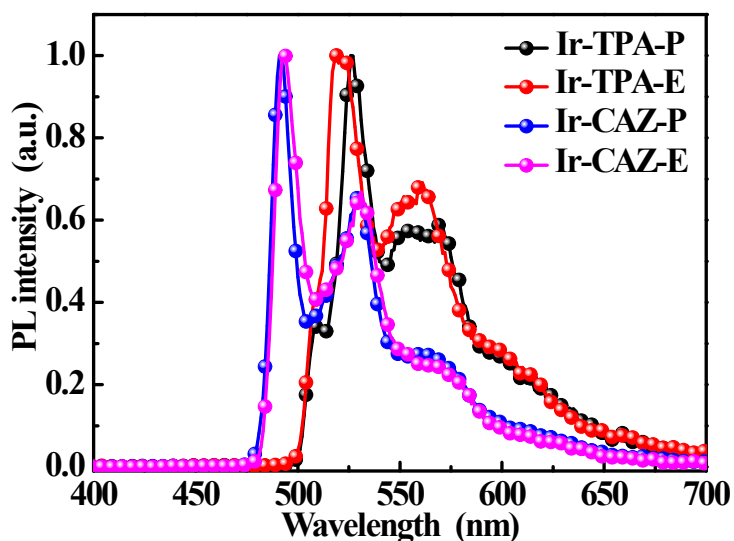
Under nitrogen atmosphere, 2-bromopyridine (1.0 equiv.), Pd(PPh<sub>3</sub>)<sub>4</sub> (5-mol% of 2-bromopyridine) and (4-(diphenylamino)phenyl)boronic acid or (4-(9H-carbazol-9-yl)phenyl)boronic acid (1.2 equiv.) were added to the mixture of toluene and 2M Na<sub>2</sub>CO<sub>3</sub>. The reaction mixture was stirred vigorously at 110 °C for 20 h. After cooling to room temperature, the reaction mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> for three times. The combined organic phase was dried over anhydrous MgSO<sub>4</sub>. After removing solvent, the residue was purified on silica gel column with CH<sub>2</sub>Cl<sub>2</sub> and hexane (6:1, v:v) as eluent. The product was obtained as solid with slight pale-yellow color.

**L-TPA:** yield 80%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ): 8.65 (d, 1H), 7.86 (d, 2H), 7.73-7.65 (m, 2H), 7.29-7.25 (m, 4H), 7.19-7.13 (m, 7H), 7.04 (t, 2H).

**L-CAZ:** yield 81%. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ): 8.76 (d, 1H), 8.25-8.22 (m, 2H), 8.16 (d, 2H), 7.85-7.80 (m, 2H), 7.71-7.67 (m, 2H), 7.48 (t, 2H), 7.45-7.41 (m, 2H), 7.32-7.28 (m, 3H).

## OLED fabrication and measurements

The pre-cleaned ITO (indium tin oxide) glass substrates were treated with ozone for 7 min. Then, poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) was deposited on the surface of the ITO glass by the spin-coating method under the condition of 3000 rpm and 60 s, to form a 45 nm thick hole injection layer. After being cured at 120 °C for 15 min in air, the emitting layer (20 nm) was obtained by spin coating the chloroform solution of each Ir(III) complexes and 4,4',4''-tris(carbazol-9-yl)-triphenylamine (TCTA) at various concentrations. The ITO substrate was dried in a vacuum oven at 50 °C for 20 min and transferred to the deposition system for organic and metal deposition. TPBi (1,3,5-tris-(N-(phenyl)-benzimidazole)-benzene) (45 nm), LiF (0.7 nm) and Al cathode (100 nm) were successively evaporated. TPBi is the electron transport layer, LiF is the electron buffer layer and Al is the cathode. The EL spectra and CIE coordinates were measured with a PR650 SpectraScan spectrometer. The  $J-V-L$  curves of the devices were recorded by using a Keithley 2400 sourcemeter and the luminance was measured using a PR650 SpectraScan spectrometer. All the experiments and measurements were carried out under ambient.



**Fig. S1.** PL spectra of the these Ir<sup>III</sup>(C<sup>^</sup>N)(P-donor ligand)Cl-type complexes in CH<sub>2</sub>Cl<sub>2</sub> at 77 K.

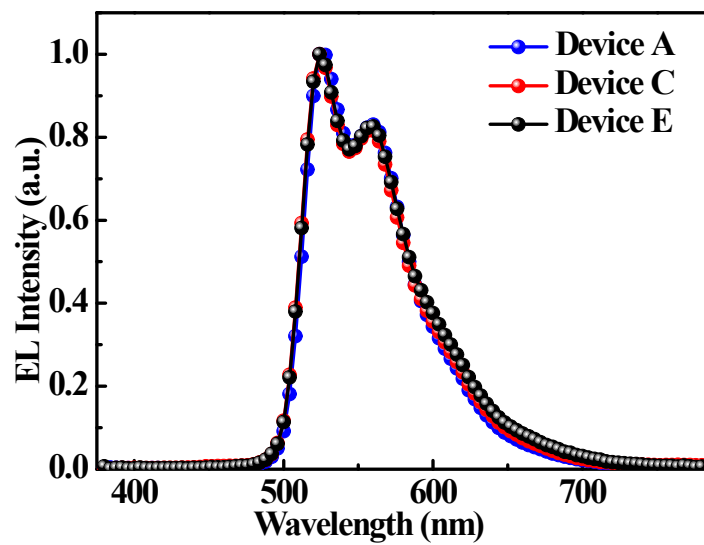


Fig. S2. EL spectra of the device A, C and E at *ca.* 10 V.

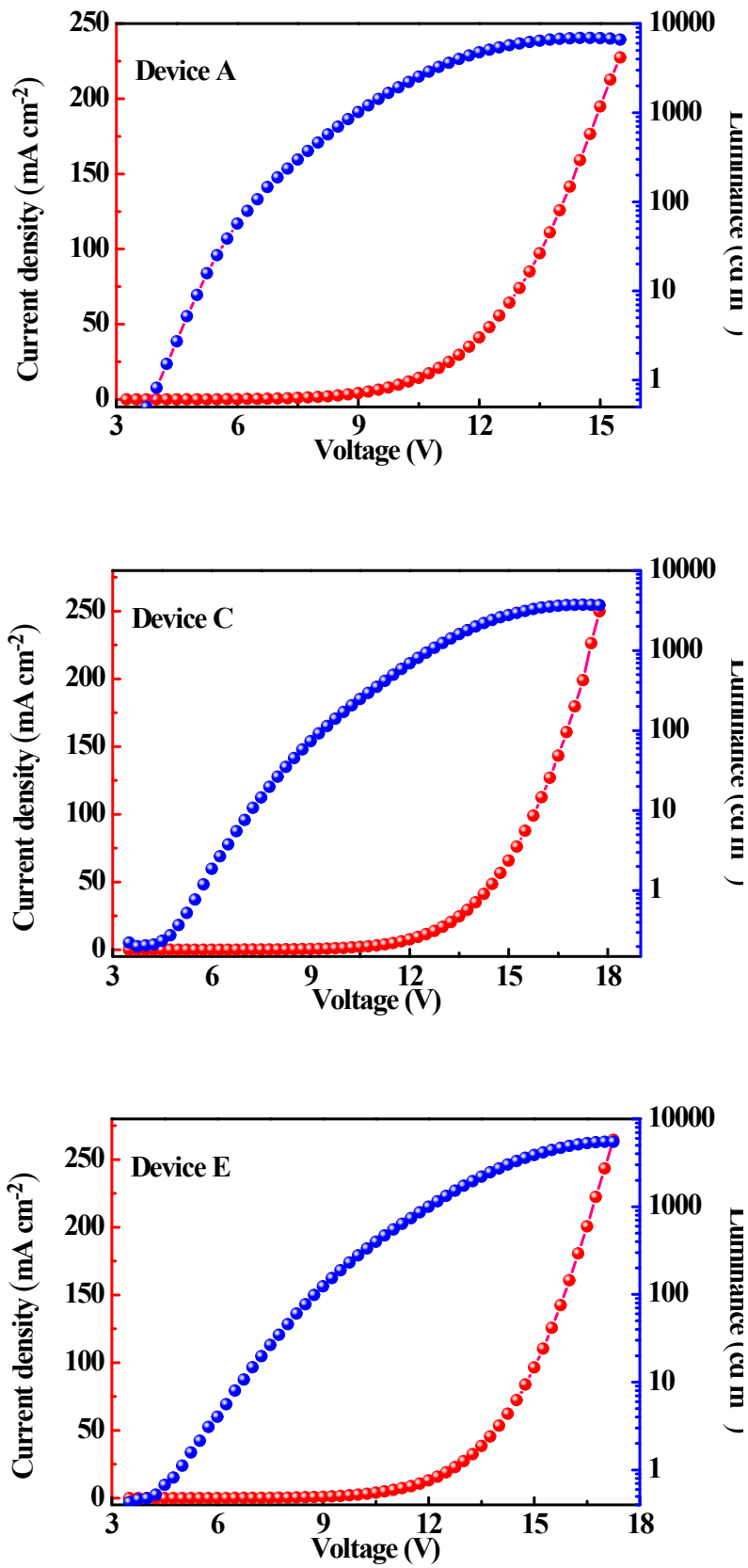
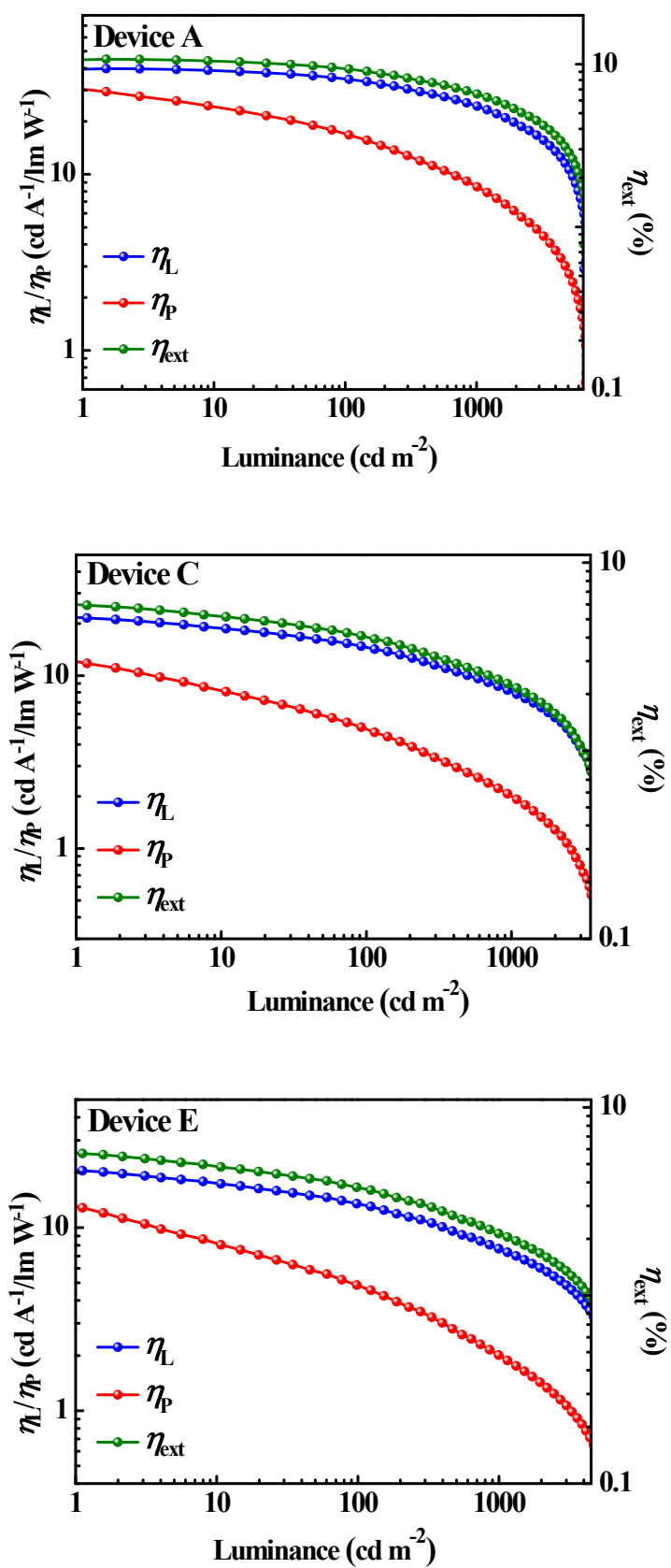


Fig. S3. Current-density–voltage–luminance ( $J$ - $V$ - $L$ ) curves for devices of A, C and E.



**Fig. S4.** Relationship between EL efficiencies and luminance for the devices of A, C and E.