Electronic Supplementary Material (ESI) for Polymer Chemistry.


# Electronic Supplementary Information

# Coordination polymers based on *bis*-$Zn^{II}$ salphen complex and functional ditopic ligands for efficient polymer light-emitting diodes (PLEDs)

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**Synthesis of B-TPA:** Under a $N_2$ atmosphere, *bis*-(pinacolato)diboron (2.2 equiv), the **Br-TPA** (1.0 equiv), KOAc (2.2 eqivs) and Pd(dppfc)$Cl_2$ (10%) were heated to 100 $^oC$ in 25 ml degassed 1,4-dioxane for 24 h. After cooling to room temperature, the mixture was extracted with dichloromethane (DCM), the organic phase was dried over anhydrous $Na_2SO_4$ and the solvent was evaporated under reduced pressure. The residue was chromatographed using DCM and petroleum ether (PE) as eluent to produce the title product as a white solid (Yield: 75%). $^1H$ NMR (400 MHz, $CDCl_3$, δ): 7.85 (s, 2H), 7.82 (d, $J$ = 4.0 Hz, 2H), 7.77 (d, $J$ = 7.6 Hz, 2H), 7.21 (t, $J$ = 8.4 Hz, 8H), 7.08 (t, $J$ = 7.6 Hz, 12H), 6.97 (t, $J$ = 7.2 Hz, 4H), 6.89 (d, $J$ = 2.2 Hz, 4H), 1.34 (d, $J$ = 4.0 Hz, 24H); $^{13}C$ NMR (100 MHz, $CDCl_3$, δ): 151.56, 147.72, 146.00, 142.73, 139.37, 134.28, 132.29, 129.18, 129.10, 124.32, 123.18, 122.59, 119.80, 83.77, 64.59, 24.88. FAB-MS: $m/z$ = 808 $[M]^+$. $C_{49}H_{34}Br_2N_2$: calcd. C 72.60, H 4.23, N 3.46; found C 72.49, H 4.08, N 3.37.

**Synthesis of L-SB:** To a solution of 1,2,4,5-benzenetetraamine tetrahydrochloride (130 mg, 0.4577 mmol) in 20 ml anhydrous methanol was added of 3,5-*di*-tert-butyl-2-hydroxybenzaldehyde (471 mg, 2.014 mmol). After 18 h continuously stirring, the yellow precipitate was collected and washed with anhydrous methanol and dried under vacuum. The yellow solid was obtained (Yield: 92%, 423 mg). $^1H$ NMR (400 MHz, $CDCl_3$, δ): 13.47 (s, 4H), 8.78 (s, 4H), 7.47 (d, $J$ = 2.4 Hz, 4H), 7.27 (d, $J$ = 2.4 Hz, 4H), 7.16 (s, 2H), 1.46 (s, 36H), 1.34 (s, 36H); $^{13}C$ NMR (100 MHz, $CDCl_3$, δ): 164.65, 158.63, 141.57, 140.50, 137.24, 128.50, 126.91, 118.32, 111.14, 35.12, 34.19, 31.45, 29.42. FAB-MS: $m/z$ = 1002 $[M]^+$. $C_{66}H_{90}N_4O_4$: calcd. C 79.00, H 9.04, N 5.58; found C 78.89, H 8.98, N 5.46.

**Synthesis of Zn-C:** To a solution of *bis*-Schiff Base compound **L-SB** (100 mg, 9.97 mmol) in 20 ml mixture of chloroform and methanol (2 : 1) was added $Zn(AcO)_2 \cdot H_2O$ (67 mg, 2.989 mmol). After stirring the mixture at room temperature for 18 h, the solvent was evaporated and the red solid was

dissolved in dichloromethane and the insoluble residue was filtered off. After evaporating dichloromethane from the filtrate, the red **Zn-C** was obtained by recrystallization in acetonitrile (Yield: 65%, 73 mg). $^1$H NMR (400 MHz, acetone-$d_6$, δ): 9.25 (s, 4H), 8.50 (s, 2H), 7.47 (d, $J$ = 4 Hz, 4H), 7.19 (d, $J$ = 2.4 Hz, 4H), 1.55 (s, 36H), 1.34 (s, 36H). FAB-MS: $m/z$ = 1126 $[M]^+$. $C_{66}H_{86}N_4O_4Zn_2$: calcd. C 70.14, H 7.67, N 4.96; found C 70.03, H 7.72, N 4.79.

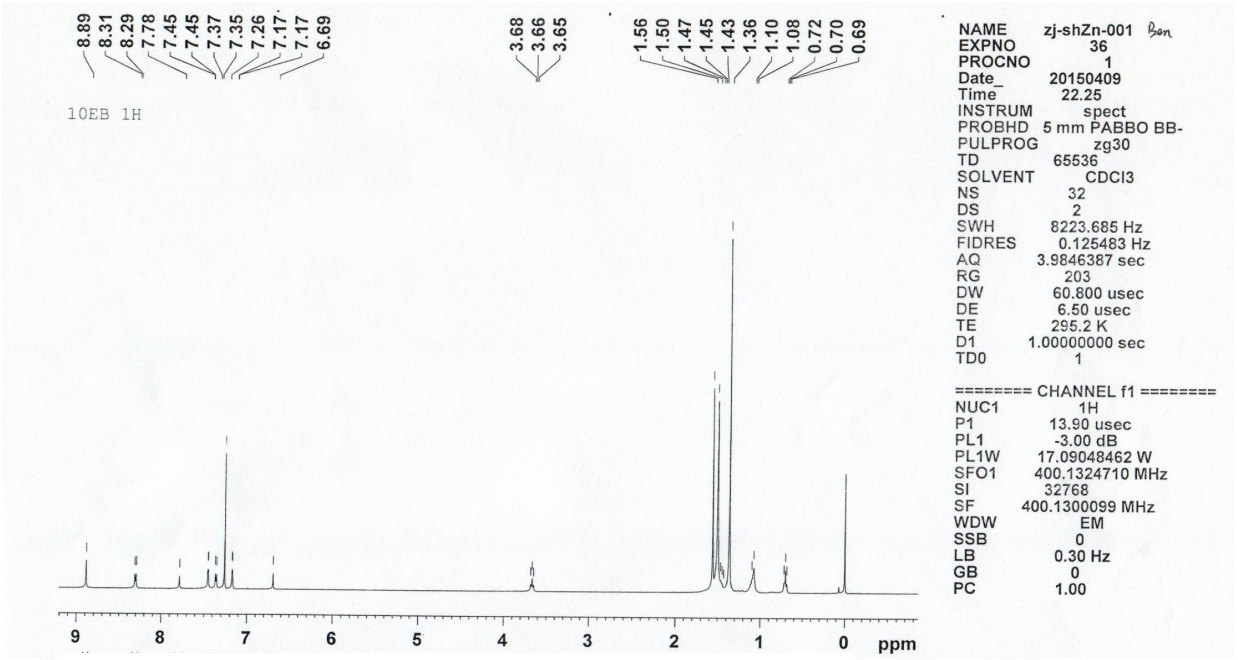


**Fig. S1** $^1$H NMR spectrum for **P-Ben**

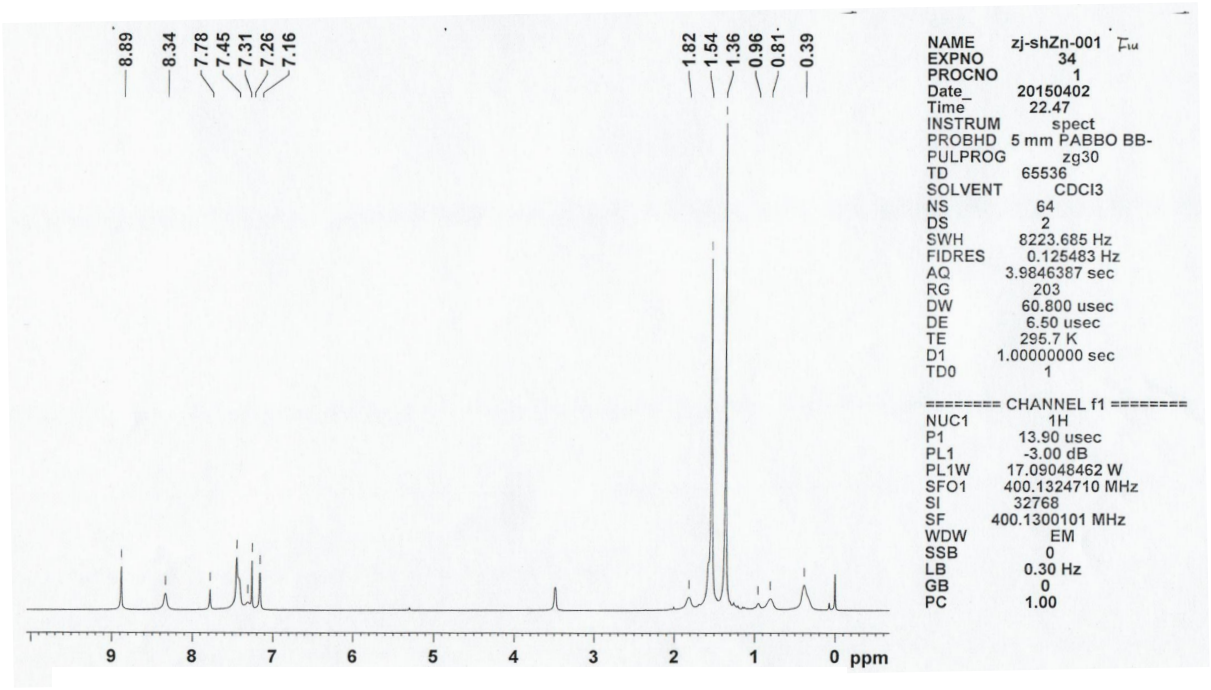


**Fig. S2** [1]H NMR spectrum for **P-Flu**

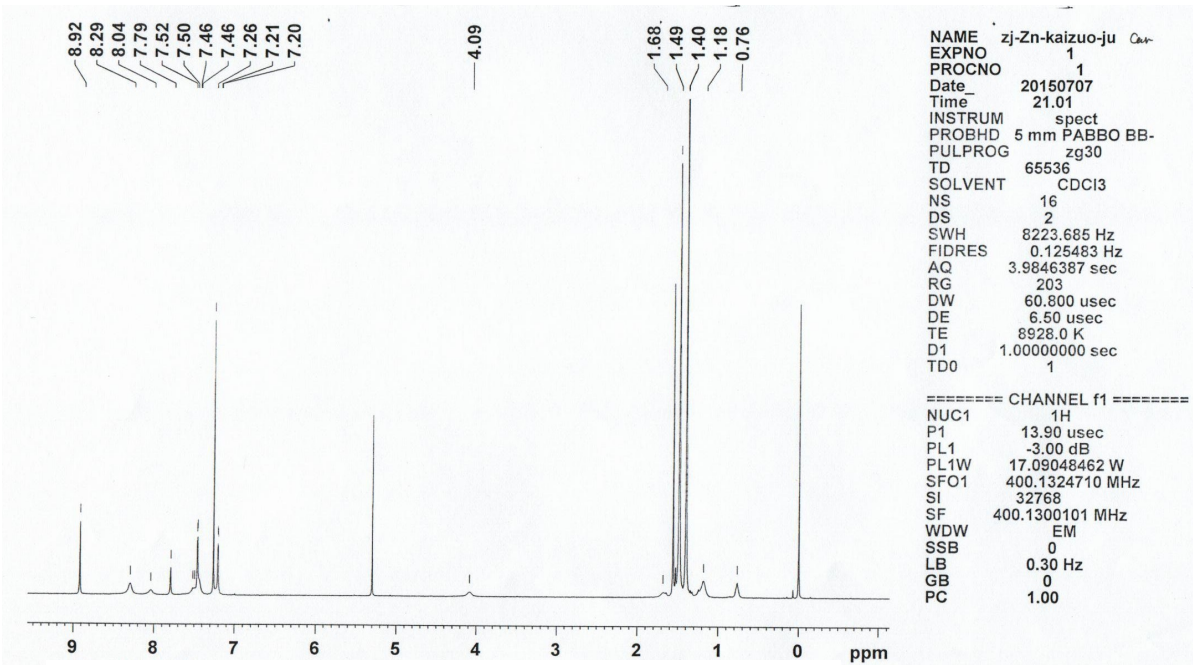


**Fig. S3** [1]H NMR spectrum for **P-Car**

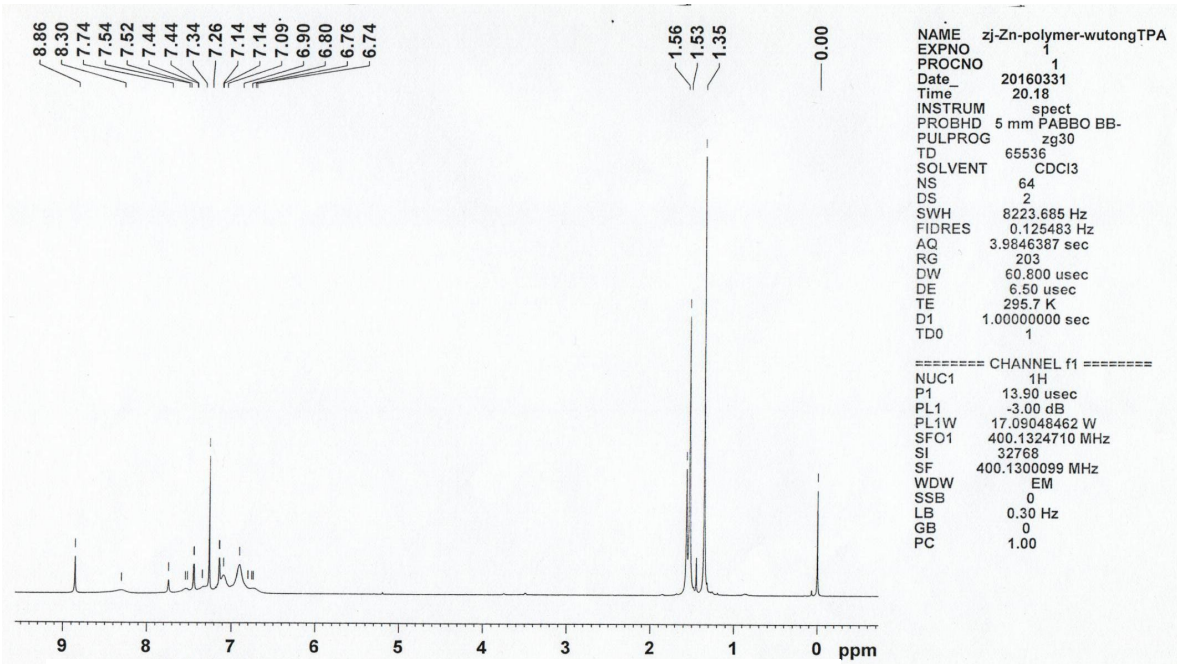


**Fig. S4** [1]H NMR spectrum for **P-TPA**

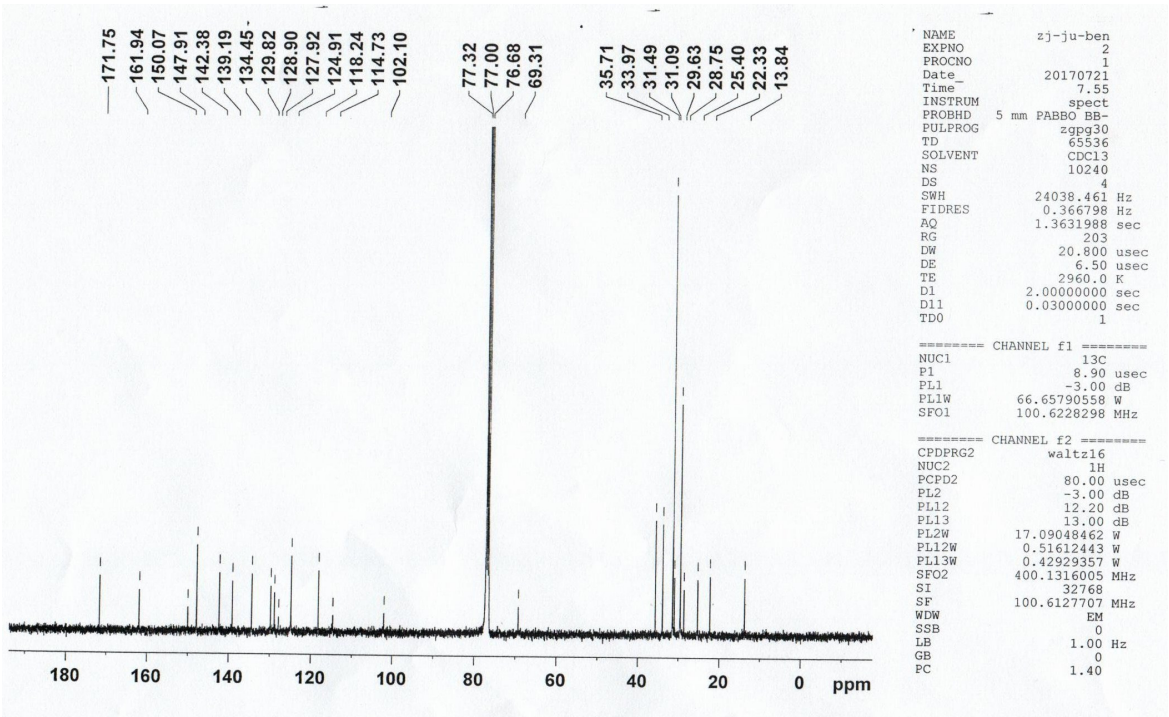


**Fig. S5** [13]C NMR spectrum for **P-Ben**

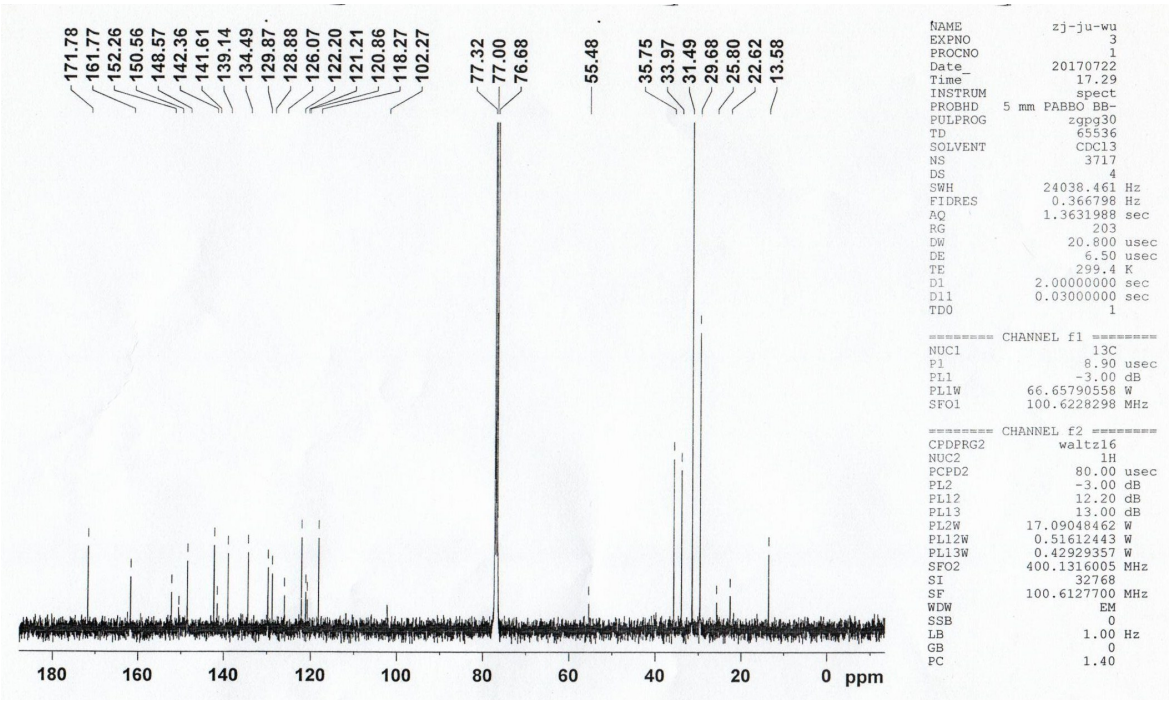


**Fig. S6** $^{13}$C NMR spectrum for **P-Flu**

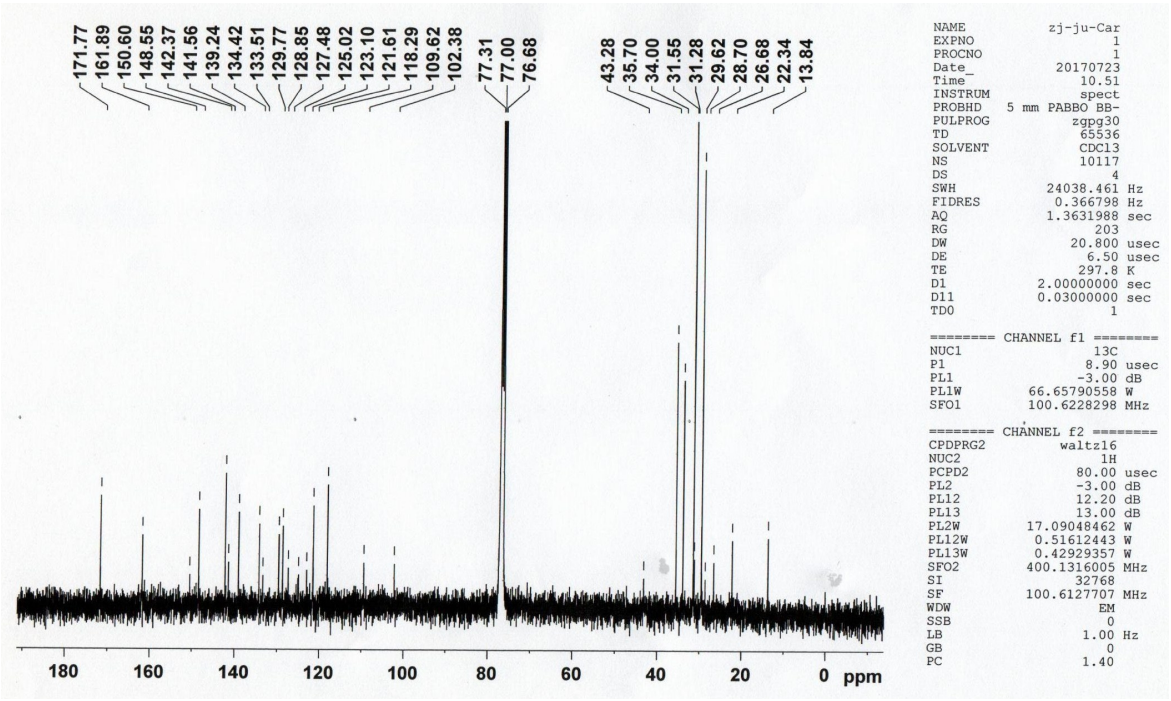


**Fig. S7** $^{13}$C NMR spectrum for **P-Car**

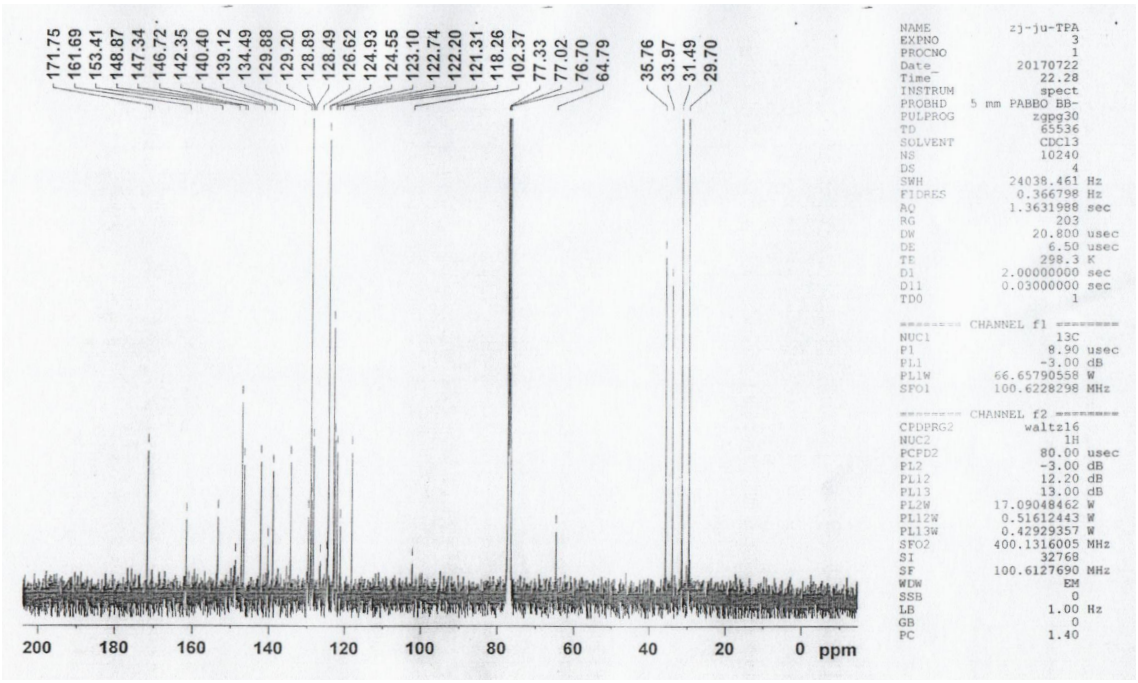


**Fig. S8** $^{13}$C NMR spectrum for **P-TPA**

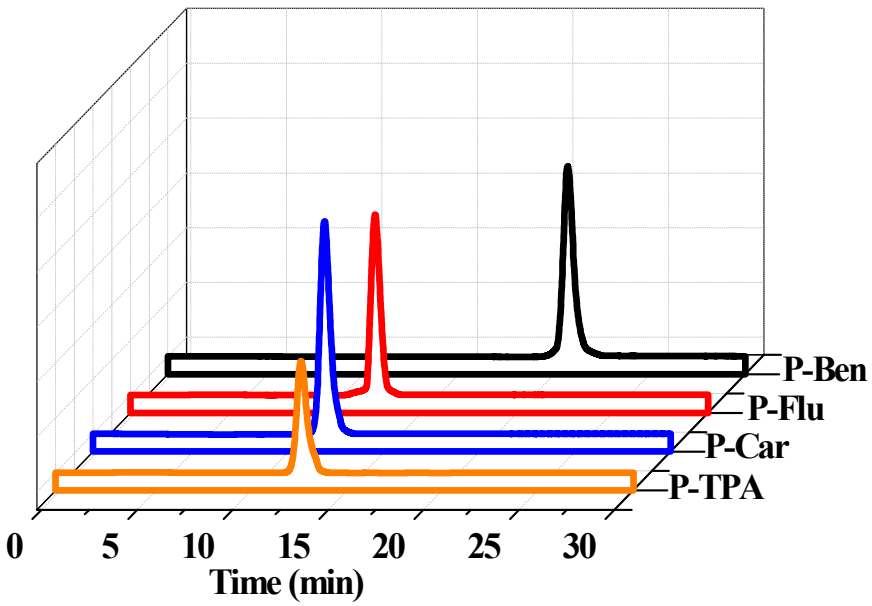


**Fig. S9** GPC curves of the *bis*-Zn$^{II}$ salphen coordination polymers.

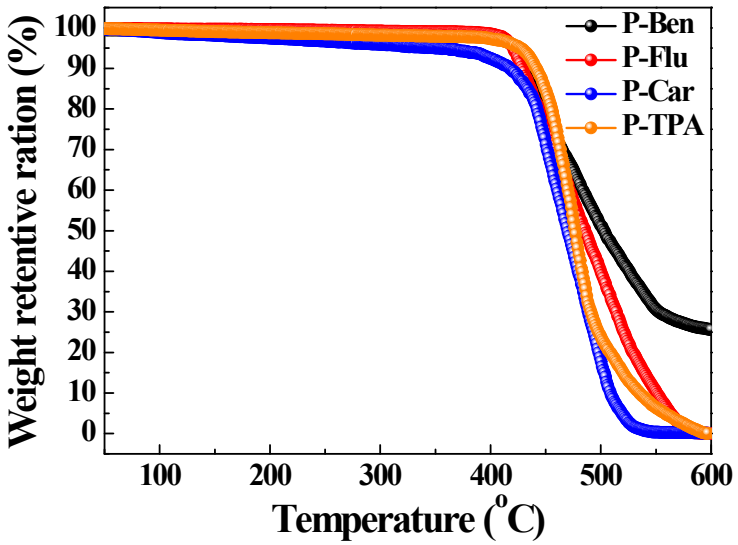


**Fig. S10** TGA curves of the *bis*-$Zn^{II}$ salphen coordination polymers.

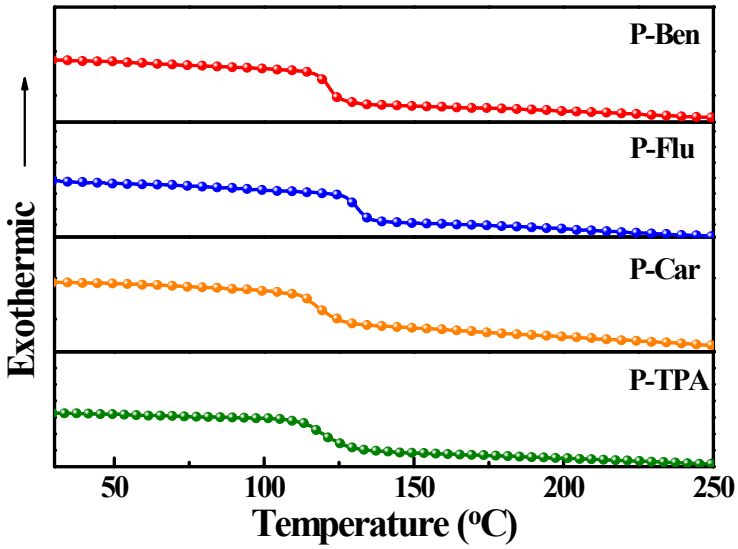


**Fig. S11** DSC curves of the *bis*-$Zn^{II}$ salphen coordination polymers.

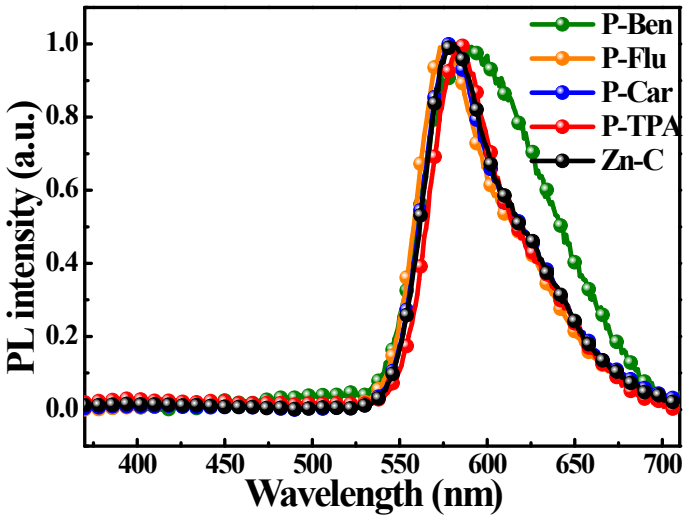


**Fig. S12** Normalized PL spectra of the *bis*-$Zn^{II}$ salphen coordination polymers and **Zn-C** in neat films on the quartz substrate.

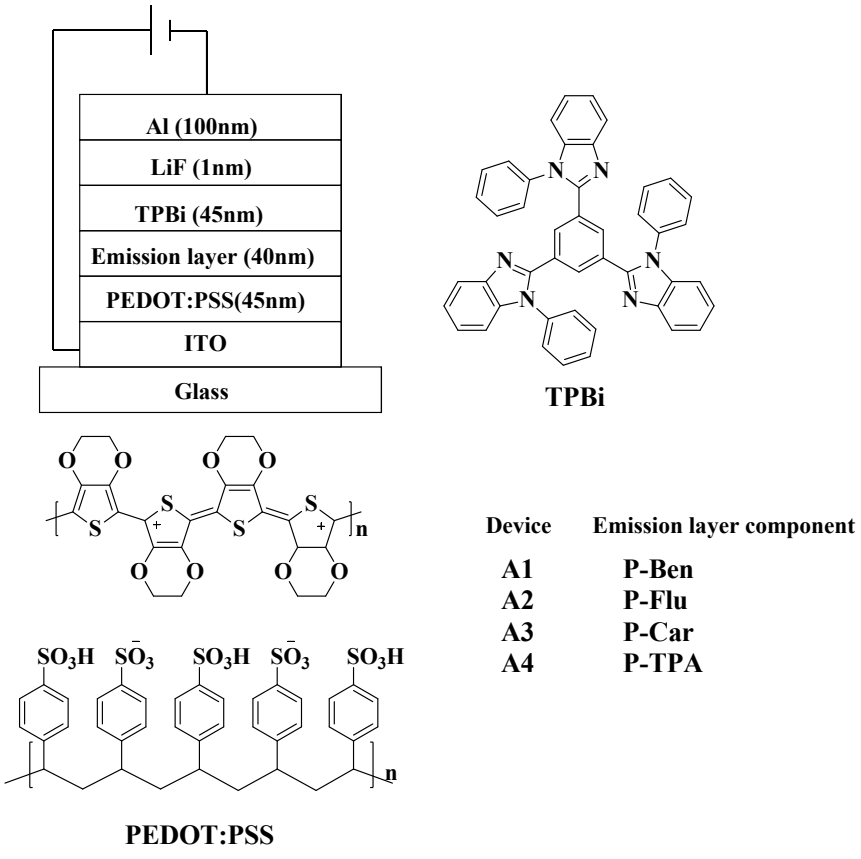


**Fig. S13** Configuration of the PLEDs made from these *bis*-$Zn^{II}$ salphen coordination polymers and the chemical structures of the functional materials involved.

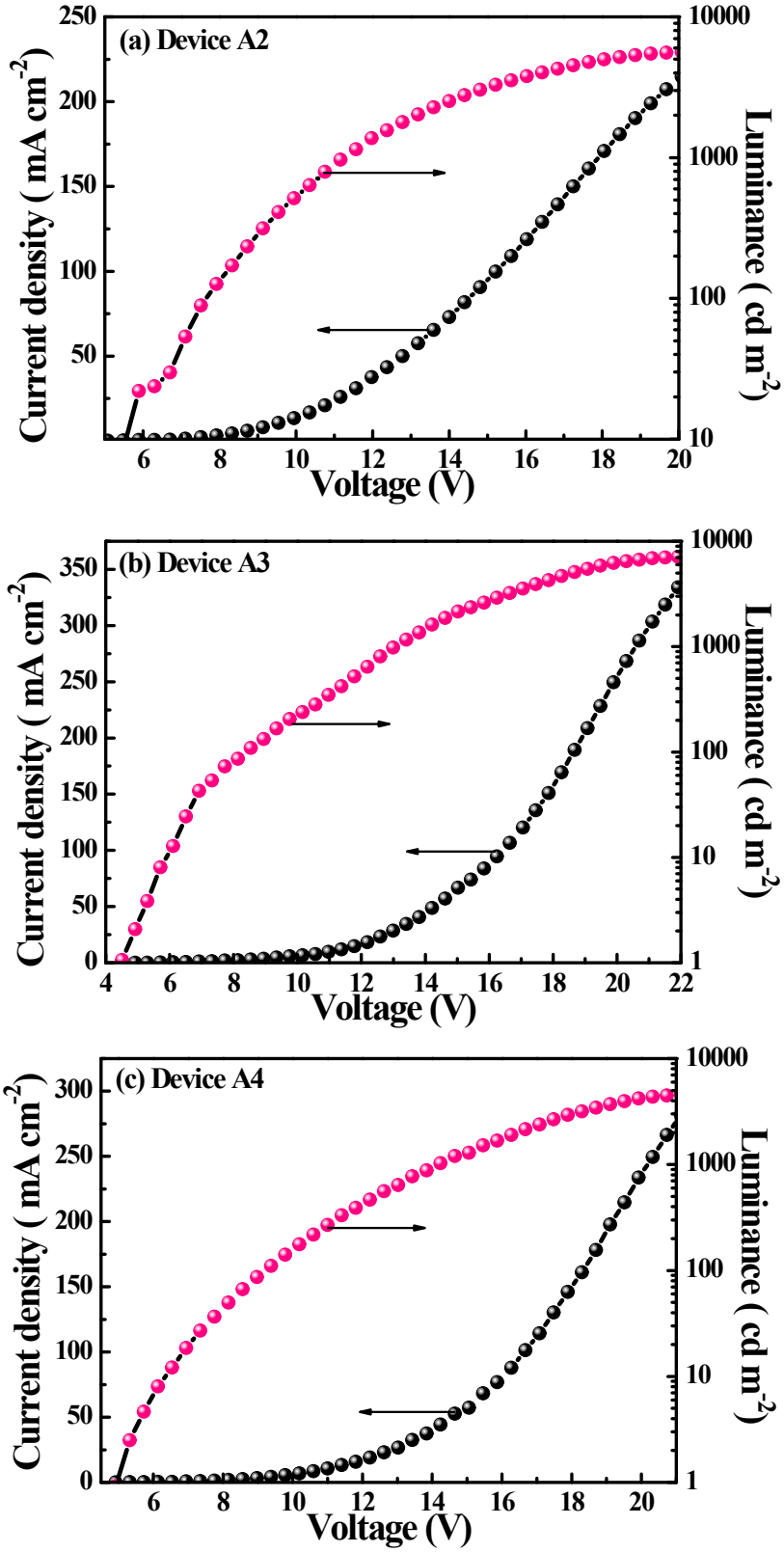


**Fig. S14** *J-V-L* curves for the devices **A2**, **A3** and **A4**.

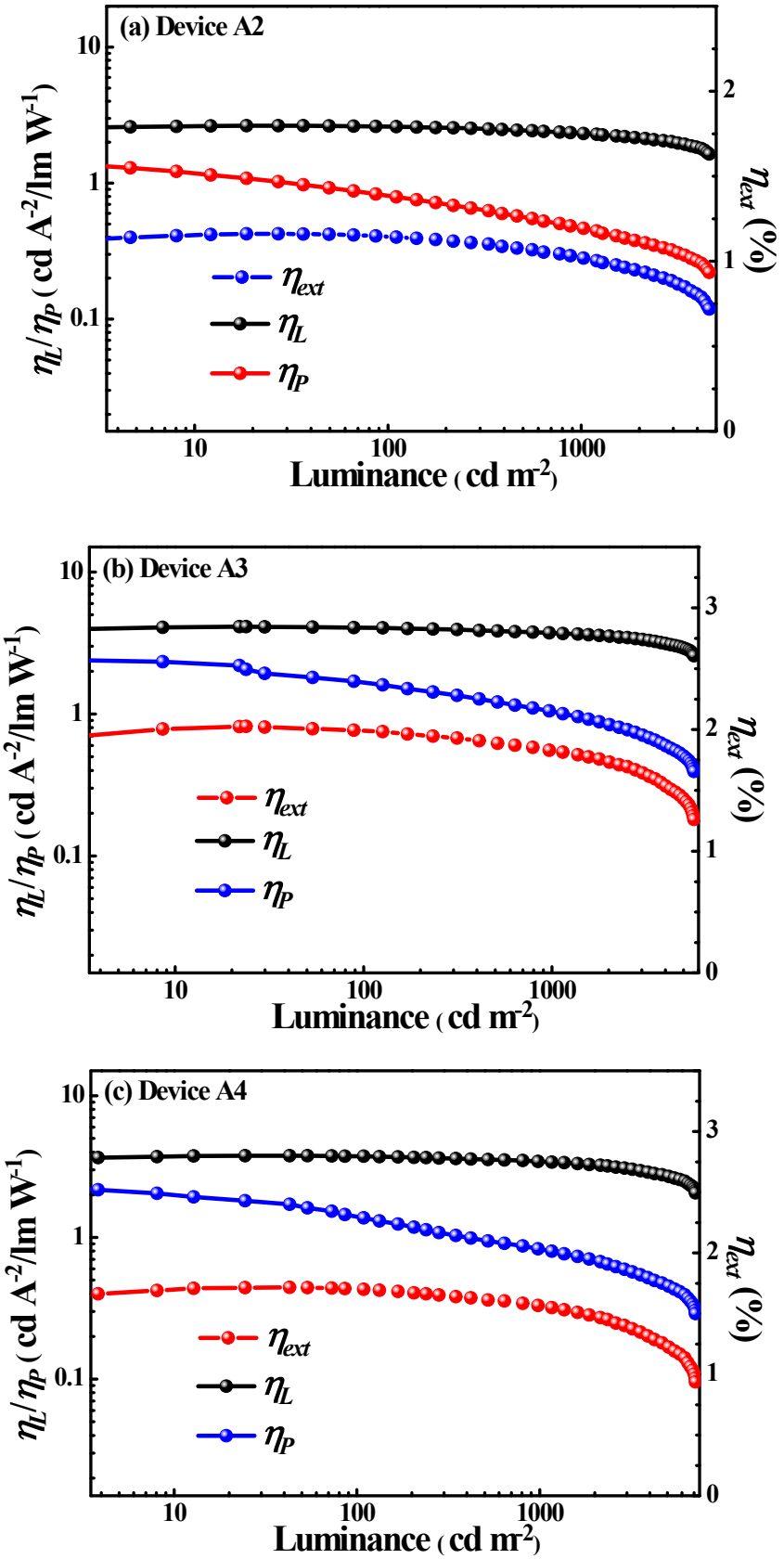


**Fig. S15** Relationship between EL efficiencies and luminance for devices **A2**, **A3** and **A4**.

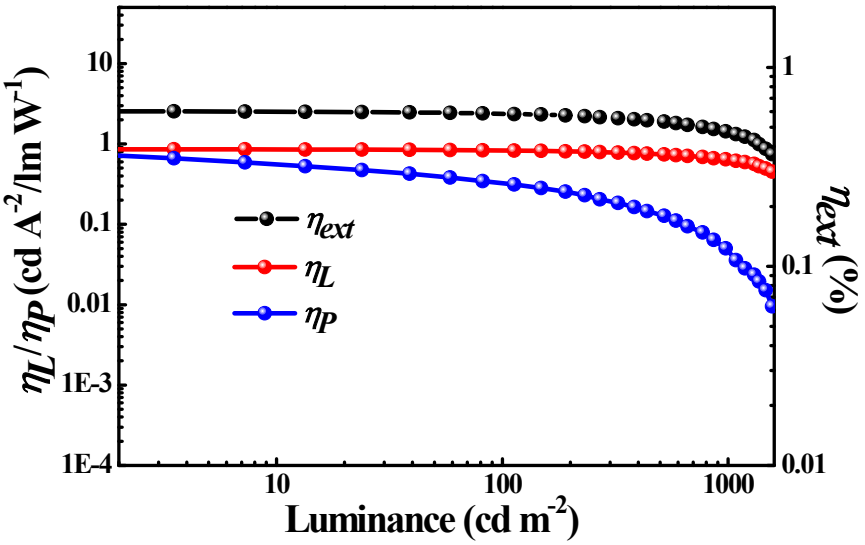


**Fig. S16** Relationship between EL efficiencies and luminance for OLED based on **Zn-C**.