

Supporting information

Highly efficient red thermally activated delayed fluorescence material based on cyano-containing planar acceptor

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Device fabrication and measurements

The OLED devices were fabricated through vacuum deposition on commercial pre-patterned ITO-coated glass substrates (ITO: 135 nm; Glass: 32 mm×32 mm×0.7 mm) with the sheet resistance of 15 Ω per square under high vacuum of 4×10^{-6} Torr. The active area of each device is 3 mm \times 3 mm. The ITO substrates were cleaned by sonication in acetone, ethanol, and deionized water for 15 min subsequently, and then dried in an oven at 110 $^{\circ}$ C and treated by UV ozone for 15 min. The deposition rates were controlled at 0.3-0.4 $\text{\AA}/\text{s}$ for HAT-CN, 0.2-0.4 $\text{\AA}/\text{s}$ for Liq, 1-2 $\text{\AA}/\text{s}$ for other organic layers and 6-8 $\text{\AA}/\text{s}$ for Al anode. The EL spectra, CIE coordinates, J - V - L curves, CE and PE of the devices were measured with a programmable spectra scan photometer (PHOTO RESEARCH, PR 655) and a constant current source meter (KEITHLEY 2400) at room temperature.

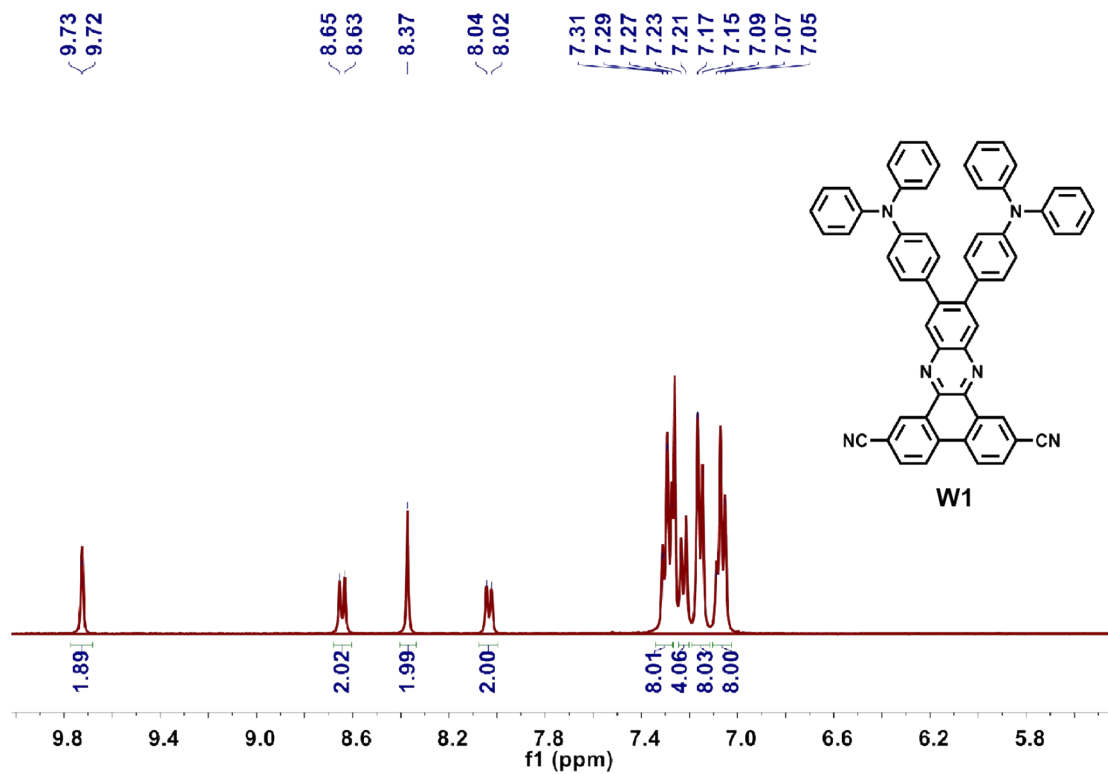


Figure S1. ¹H NMR spectrum of W1.

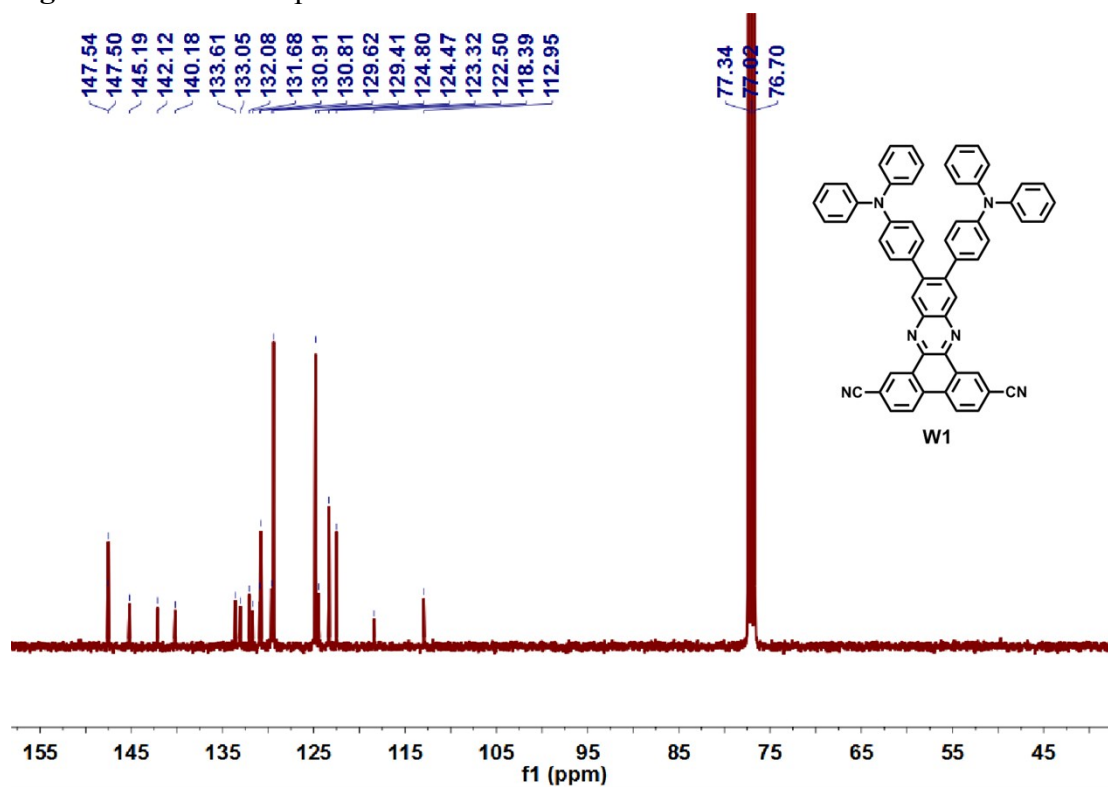


Figure S2. ¹³C NMR spectrum of W1.

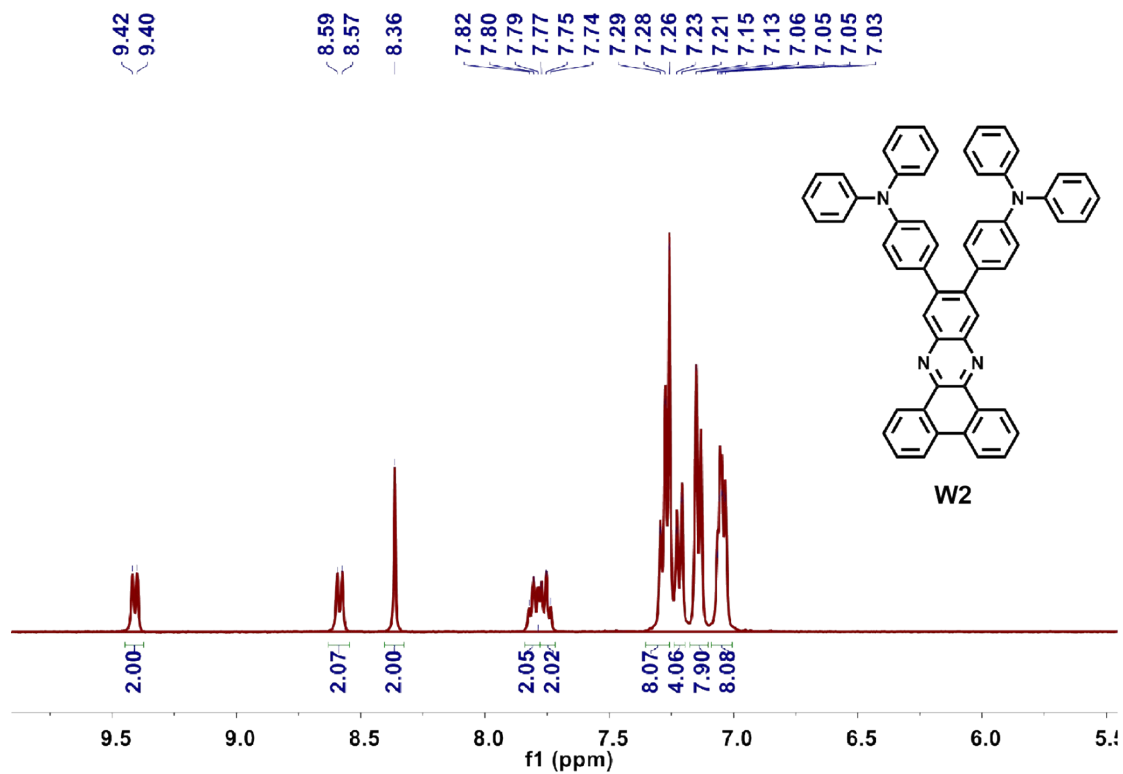


Figure S3. ^1H NMR spectrum of W2.

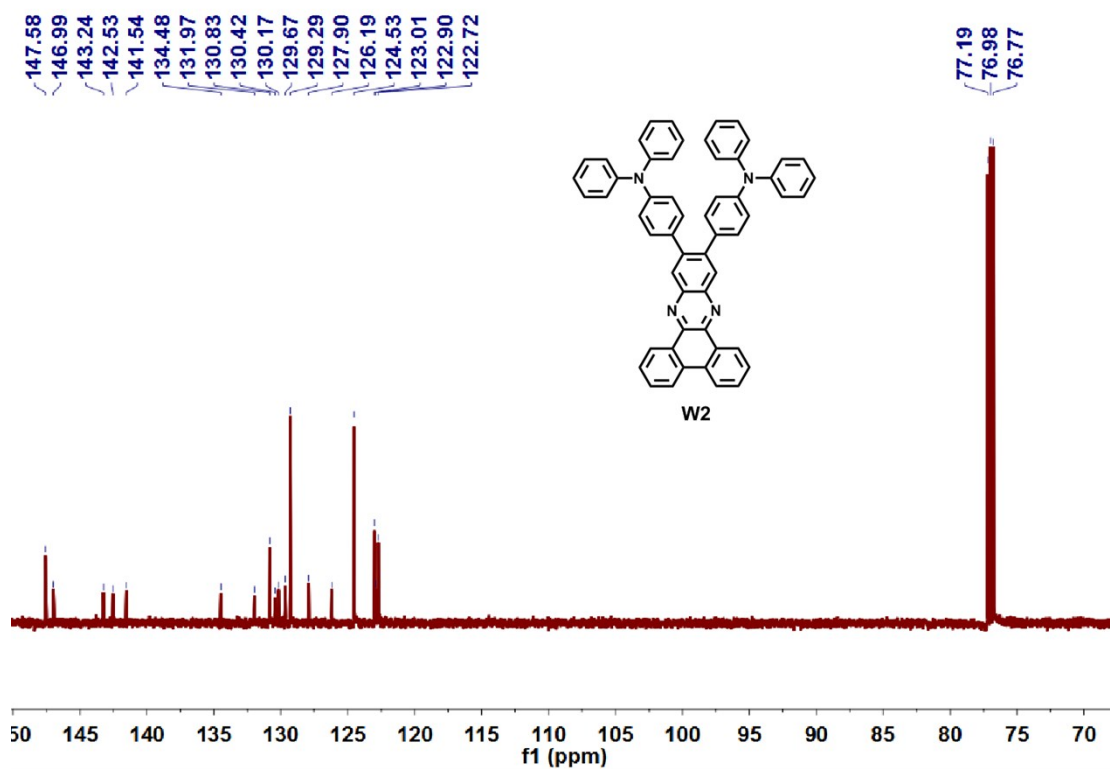


Figure S4. ^{13}C NMR spectrum of W2.

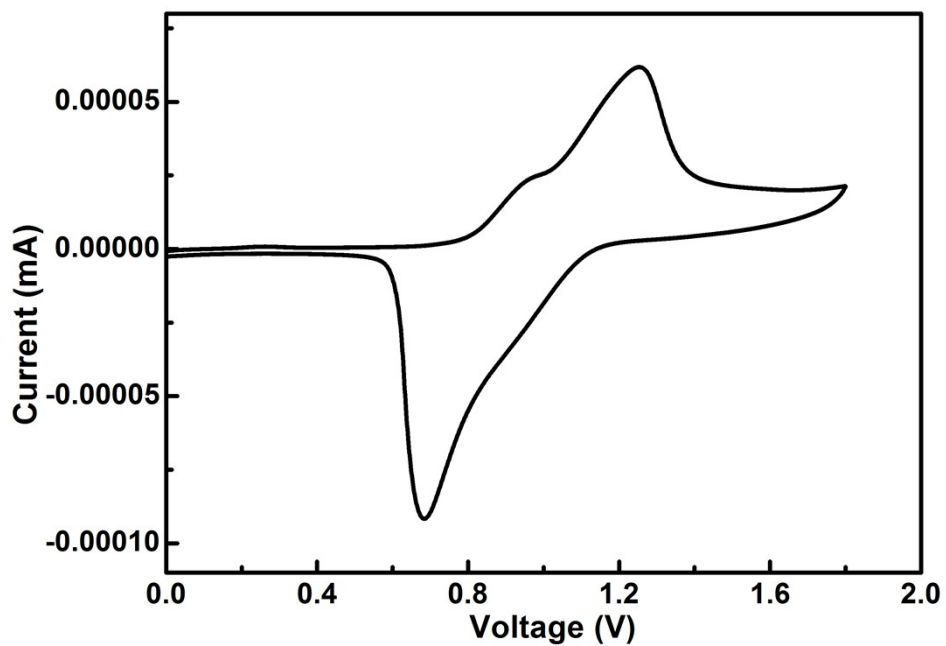


Figure S5. Cyclic voltammogram of W1 measured in THF for oxidation at room temperature.

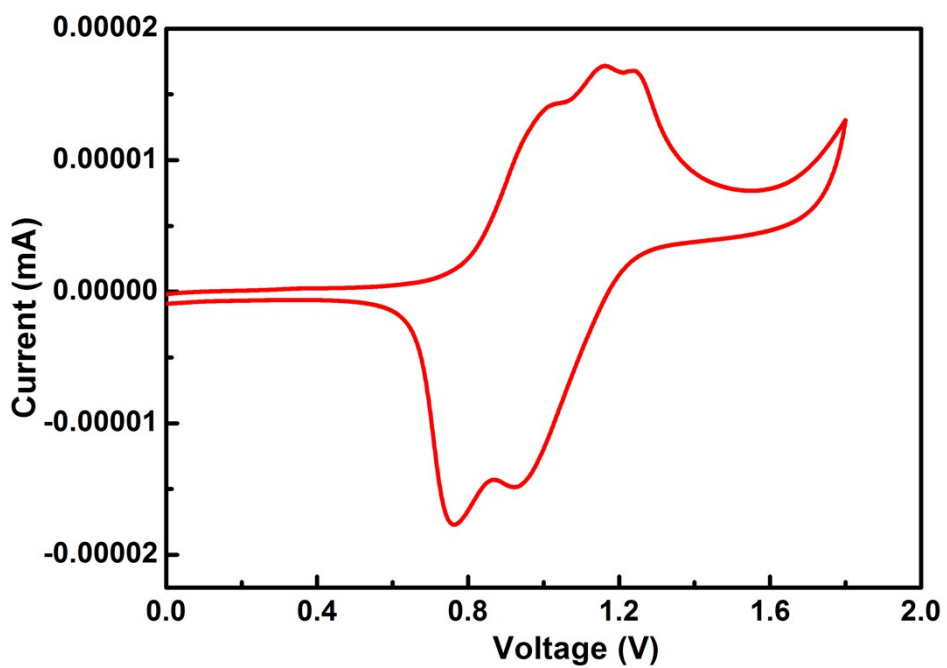


Figure S6. Cyclic voltammogram of W2 measured in THF for oxidation at room temperature.

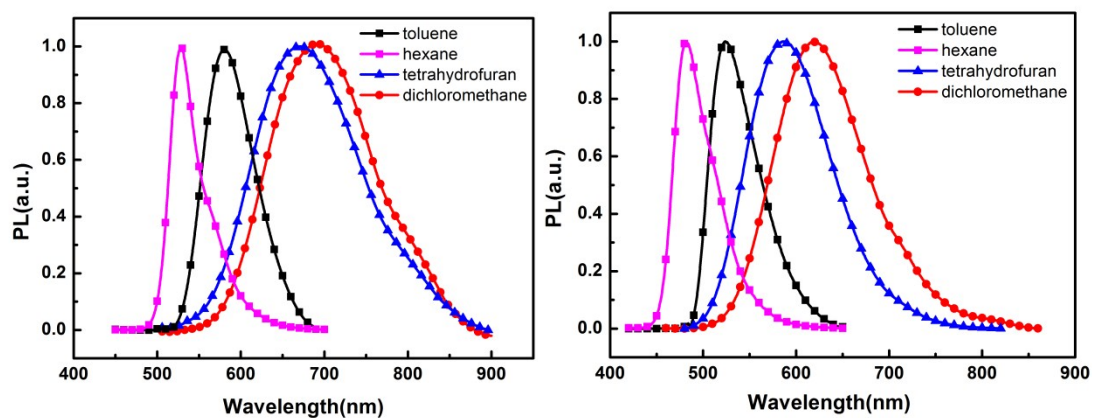


Figure S7. Normalized PL spectra of W1 (left) and W2 (right) in different solvents.

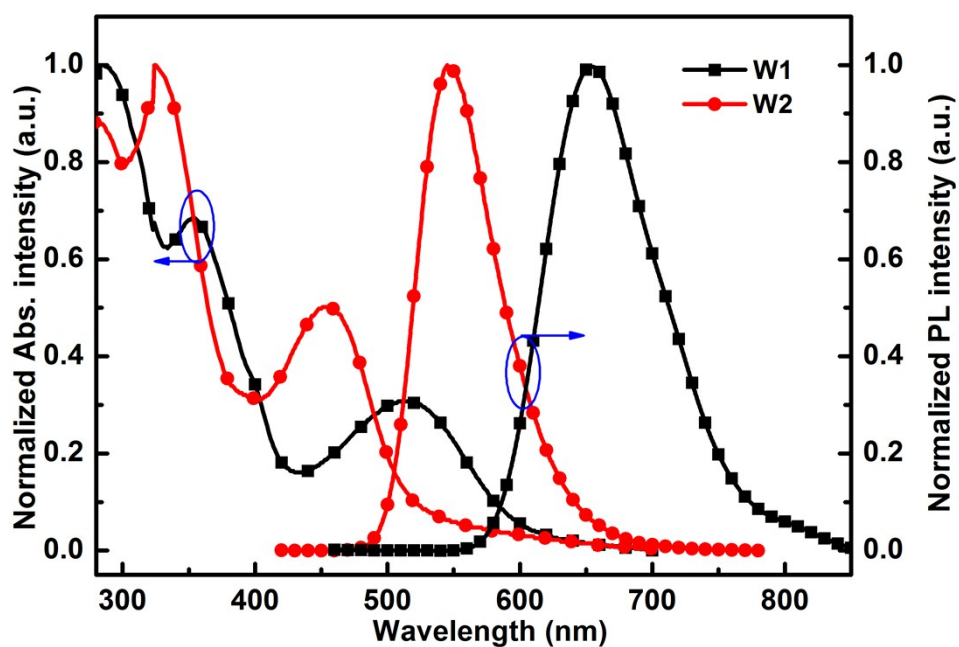


Figure S8. Normalized UV-vis absorption and PL spectra of W1&W2 neat film.

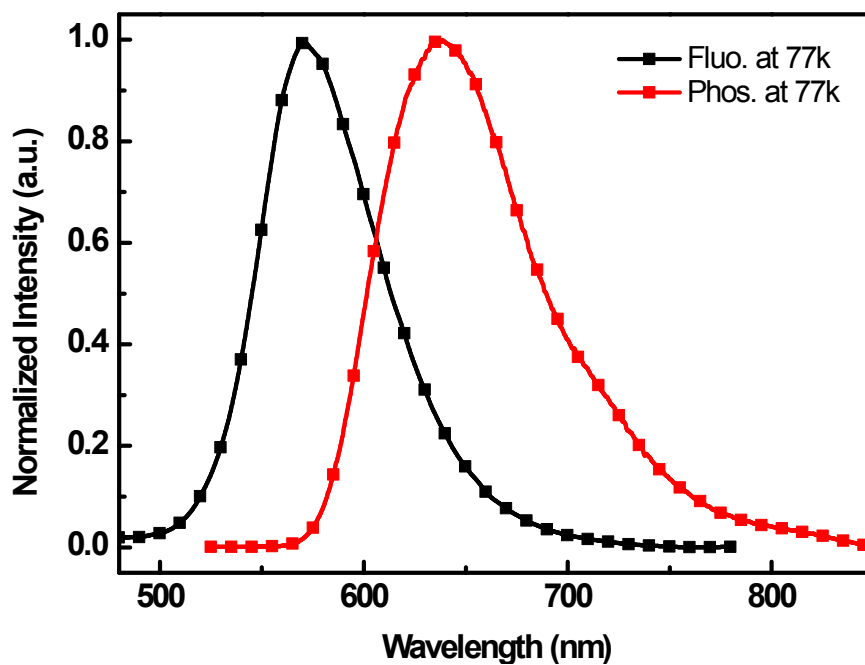


Figure S9. Fluorescence and phosphorescence spectra of W1 in toluene at 77 K.

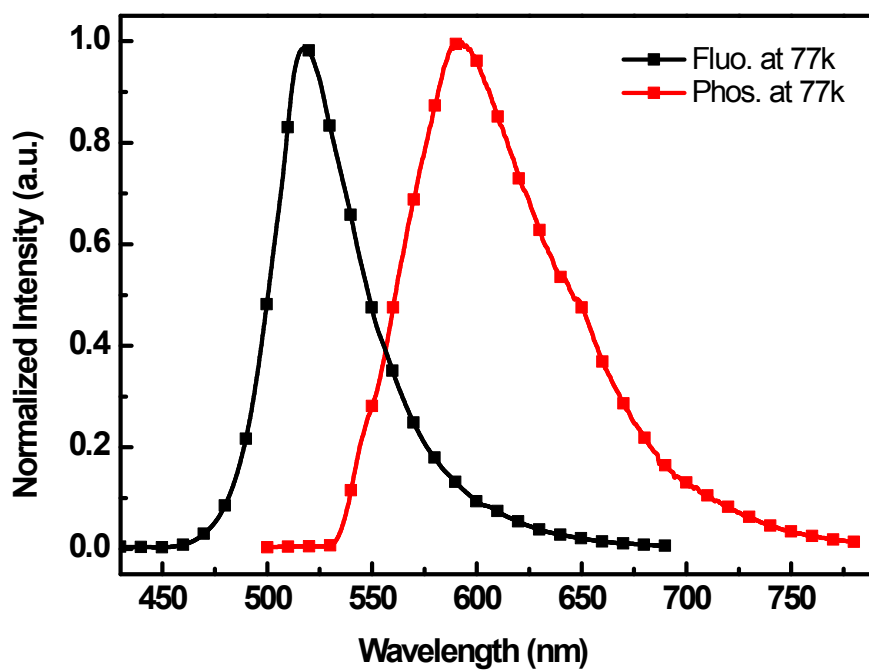


Figure S10. Fluorescence and phosphorescence spectra of W2 in toluene at 77 K.

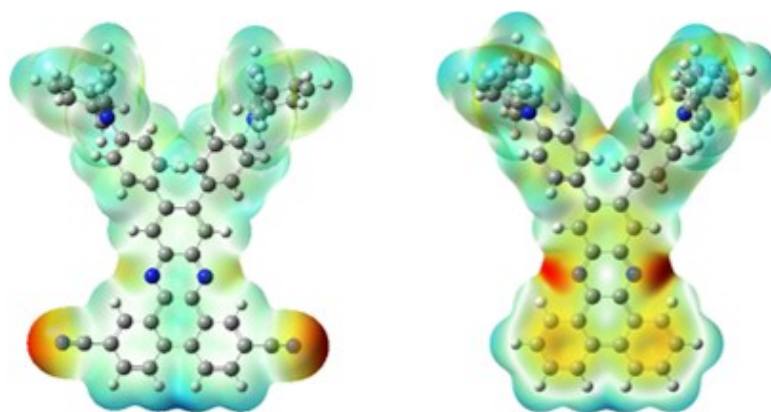


Figure S11. Isosurface of **W1** and **W2** mapped with electron static potential distribution calculation.

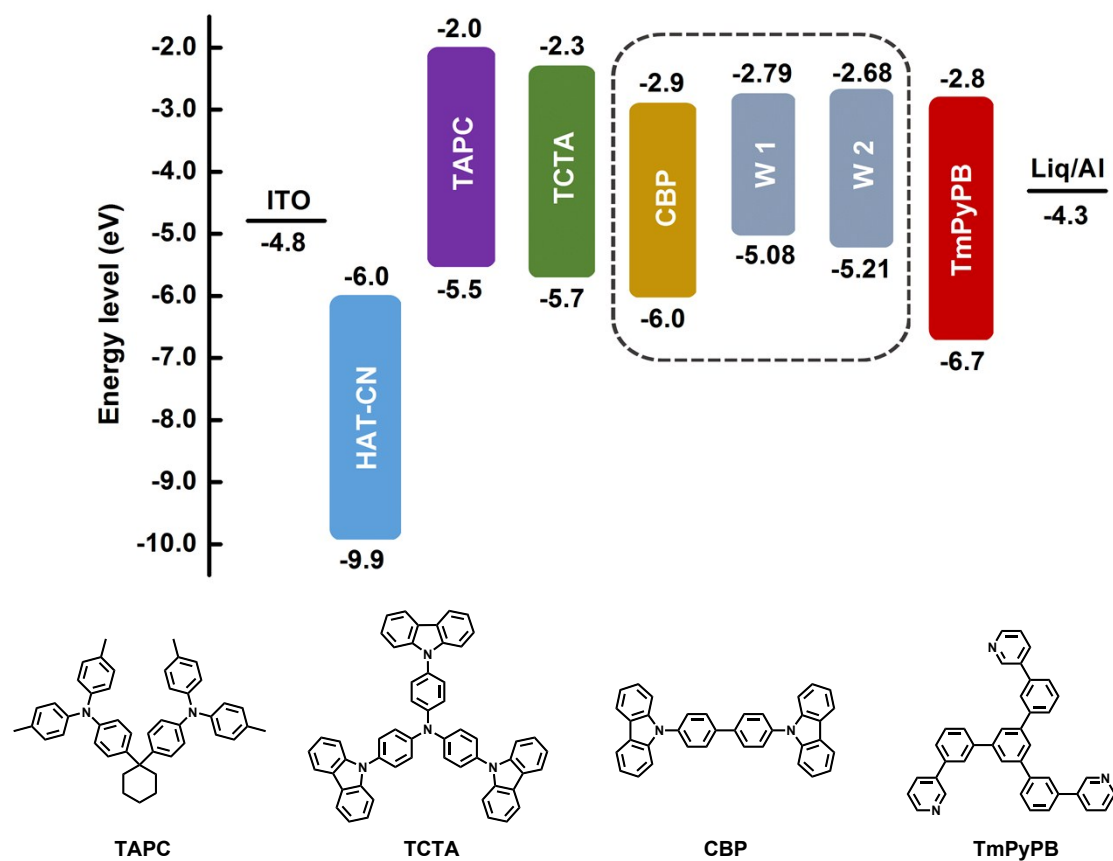


Figure S12. Energy level diagram and molecular structures of materials used in W1/W2 based device.

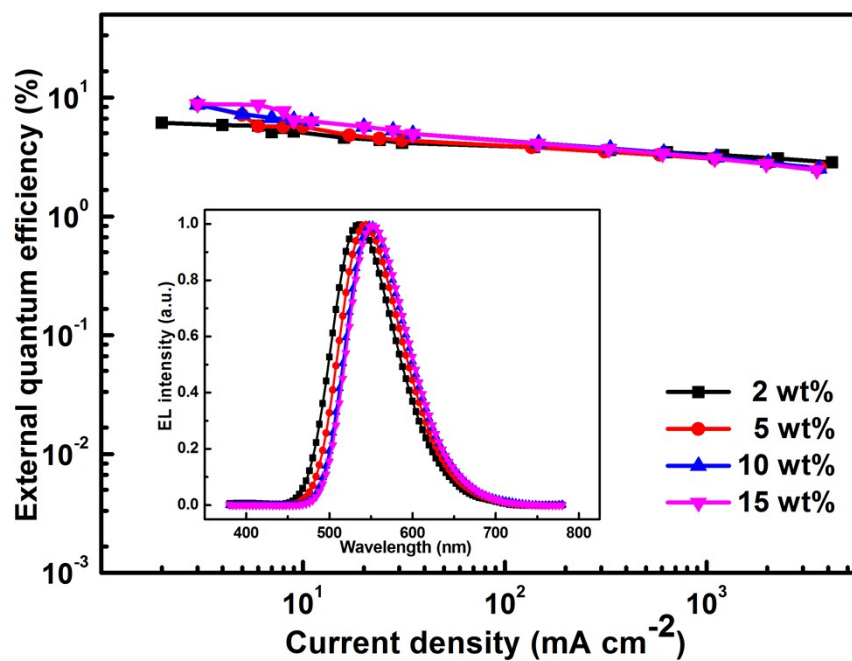


Figure S13. EQE-current density curve of W2 (inset: EL spectra at 5 mA cm⁻²).

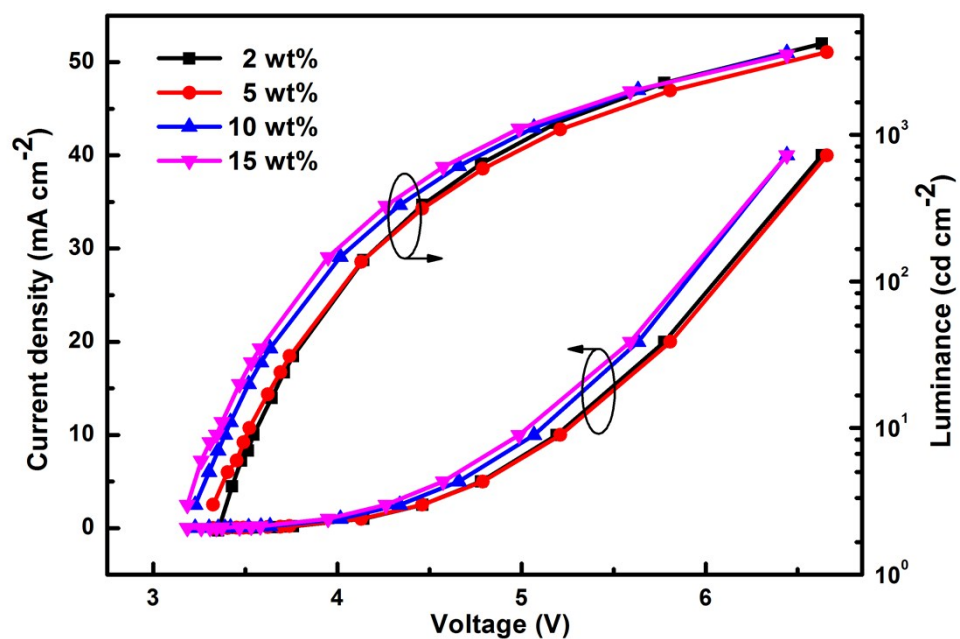


Figure S14. Current density -voltage-luminance (J - V - L) characteristics of the doped OLEDs based on W2.

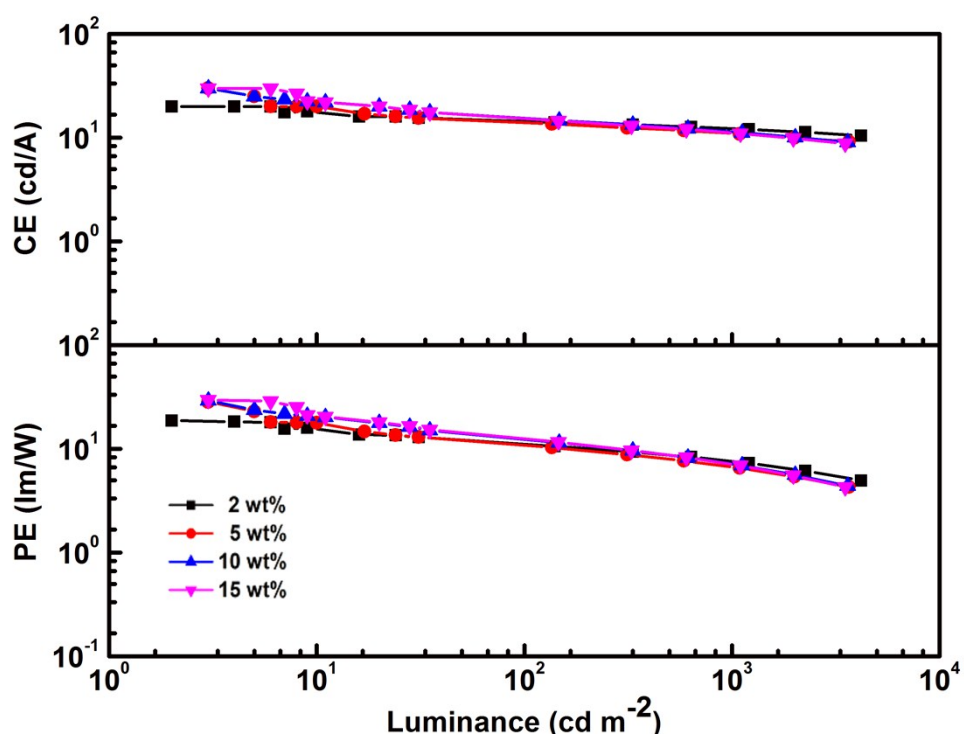


Figure S15. Power/Current Efficiency vs. Luminance relationships of W2-based device.

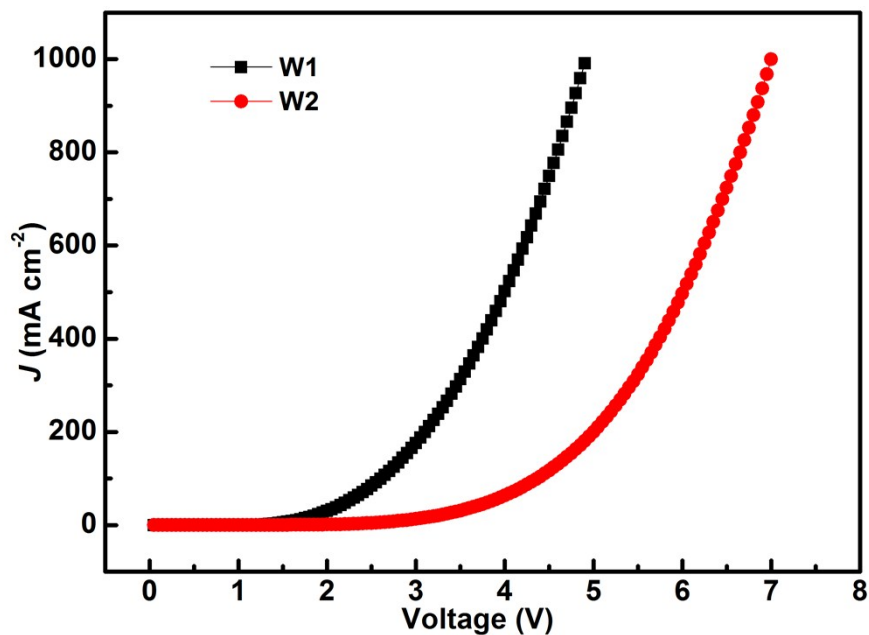


Figure S16. Current density (J)-voltage relationship of electron-only devices. Device structures: ITO/Liq (2 nm)/W1 or W2 (100 nm)/Liq (2 nm)/Al.

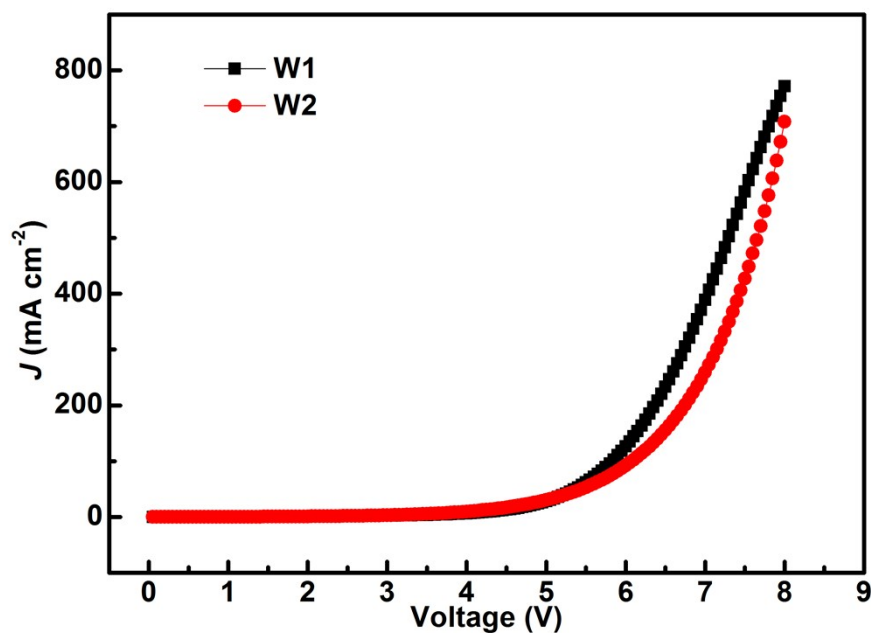


Figure S17. Current density (J)-voltage relationship of hole-only devices. Device structures: ITO/HAT-CN (10 nm)/W1 or W2 (100 nm)/HAT-CN (10 nm)/Al.

Table S1. Electroluminescence performance of **W2** doped device.

| Doping conc. wt% | V ^[a] (V) | CE ^[b] [cd/A] | PE ^[b] [lm/W] | EQE ^[b] [%] | CIE ^[c] (x,y) | λ_{EL} ^[d] nm |
|---------------------|---------------------------|-----------------------------|-----------------------------|---------------------------|-----------------------------|-------------------------------------|
| 10% | 3.86 | 30/16/11 | 29.20/13.02/7.25 | 8.69/4.38/3.20 | 0.43, 0.55 | 556 |
| 15% | 3.79 | 30/16/11 | 29.59/13.21/7.22 | 8.84/4.48/3.16 | 0.44, 0.54 | 560 |

^[a] Voltage at 100 cd m⁻².

^[b] Maximum/luminance at 100/luminance at 1000 cd m⁻².

^[c] Commission Internationale de L'Eclairage coordinates.

^[d] Measured at 5 mA cm⁻².