



## Supporting Information

for

### **Thienothiophene-based organic light-emitting diode: synthesis, photophysical properties and application**

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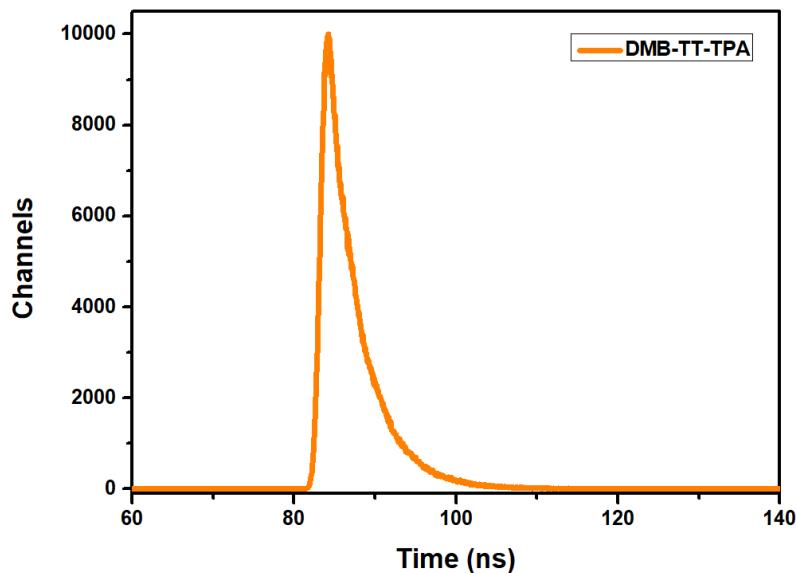
*Beilstein J. Org. Chem.* **2023**, *19*, 1849–1857. doi:10.3762/bjoc.19.137

**General experimental device methods, life time spectra,  
theoretical computation data,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra**

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## 1. Fluorescence lifetime

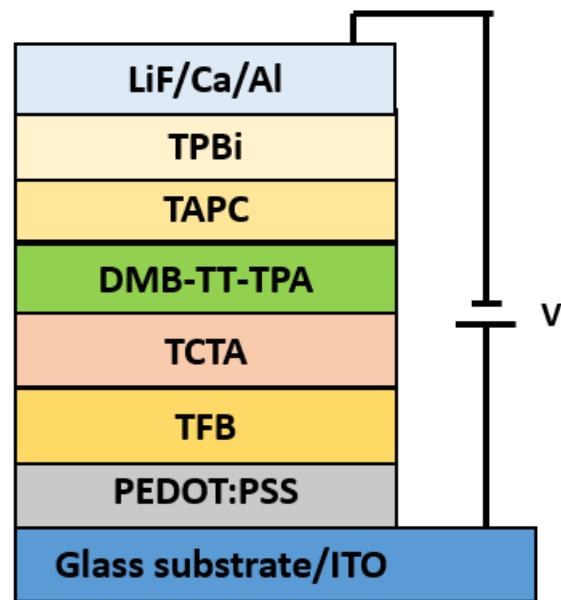


**Figure S1:** Fluorescence lifetime decay pattern of the DMB-TT-TPA (8).

## 2. General experimental device methods

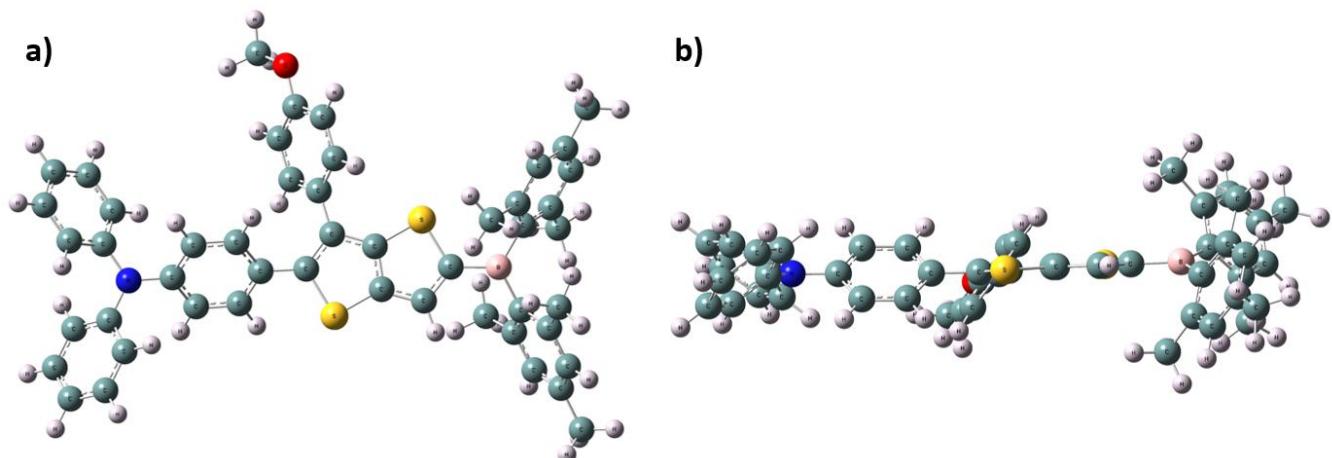
TFB (Cambridge Display Technology Ltd.) solution was prepared by dissolving TFB in toluene in 2 mg/mL concentration. The active layer solution was prepared by controlling the host material concentration fixed at 15 mg/mL and blending the emitter at 10 wt % in chlorobenzene. Prepatterned ITO substrates were rinsed in an ultrasonic bath with acetone, isopropyl alcohol, Hellmanex III, and deionized water before deposition of top layers. PEDOT:PSS and TFB were deposited on ITO sequentially via spin-coating at 2500 and 1000 rpm, respectively. Then, the prepared active layer was spin-coated on annealed TFB (180 °C for 1 h in a nitrogen glovebox) at 2000 rpm to form a 50 nm film. Afterwards, TPBi, LiF, and Ca/Ag were thermally evaporated onto the organic layer under vacuum level of  $\approx 5 \times 10^{-7}$  mbar. J–V–L characterization (pixel area = 0.045 cm<sup>2</sup>) was performed using a Keithley 2400 and Konica Minolta LS-110 Luminance Meter. OLED emission profile was assumed to be Lambertian. The EL

spectrum was measured using an Ocean Optics USB 2000 charge-coupled device spectrophotometer.

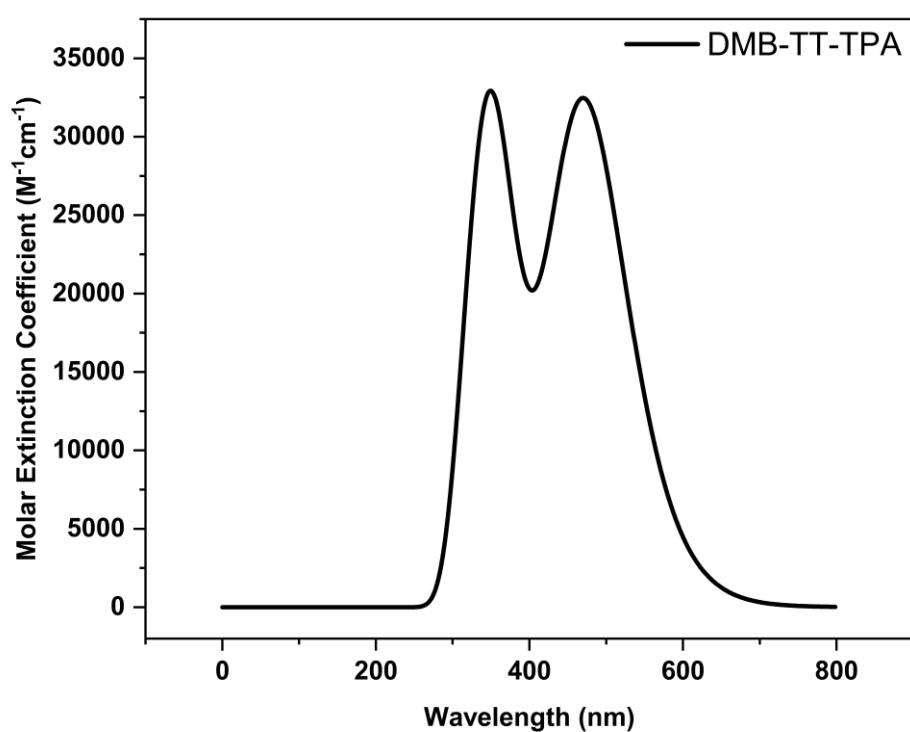


**Figure S2:** Schematic illustration of the device configuration.

### 3. Computational data

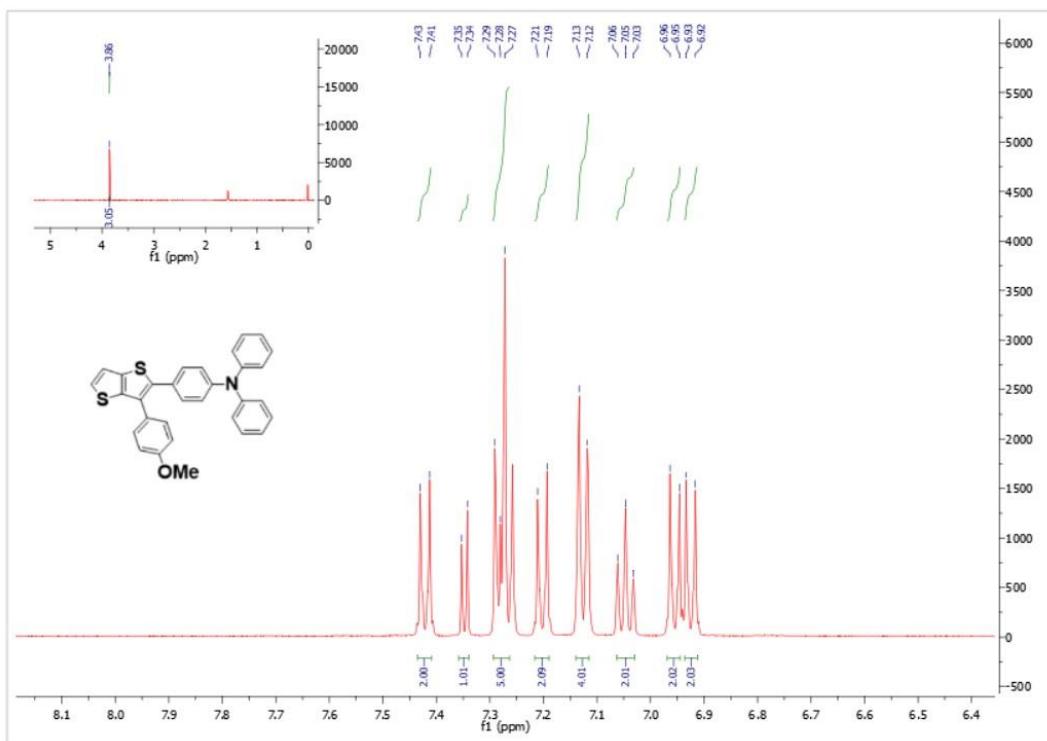


**Figure S3:** Optimized geometry of DMB-TT-TPA (8) of a) top view and b) side view.

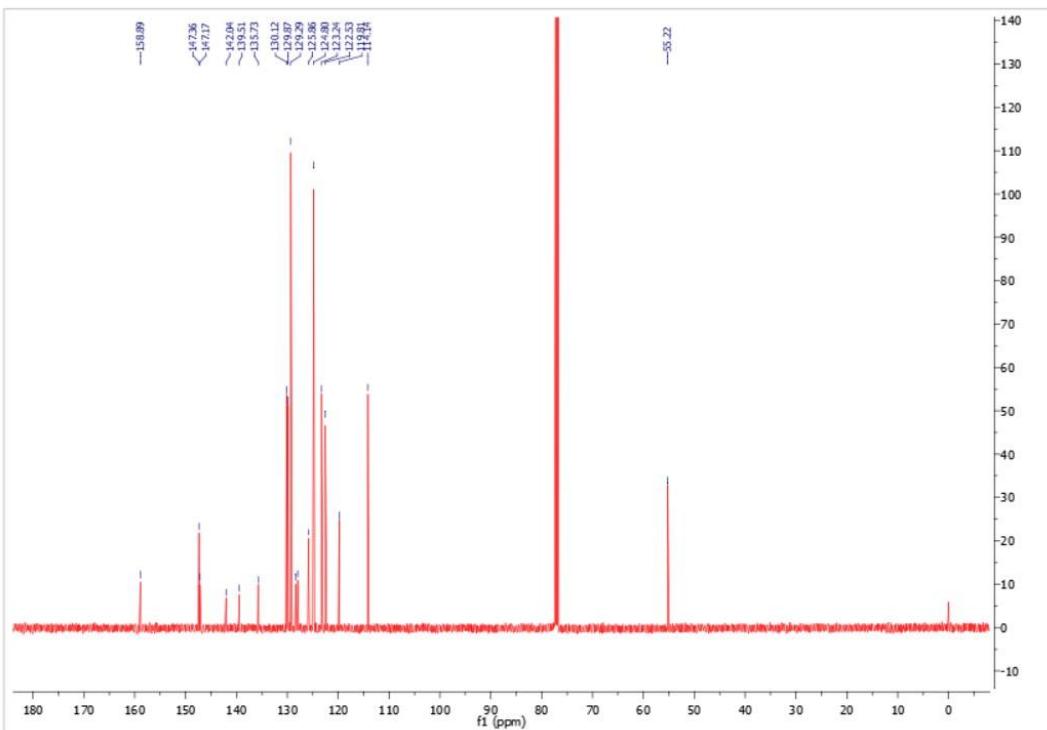


**Figure S4:** Theoretical UV–vis spectrum of DMB-TT-TPA (8).

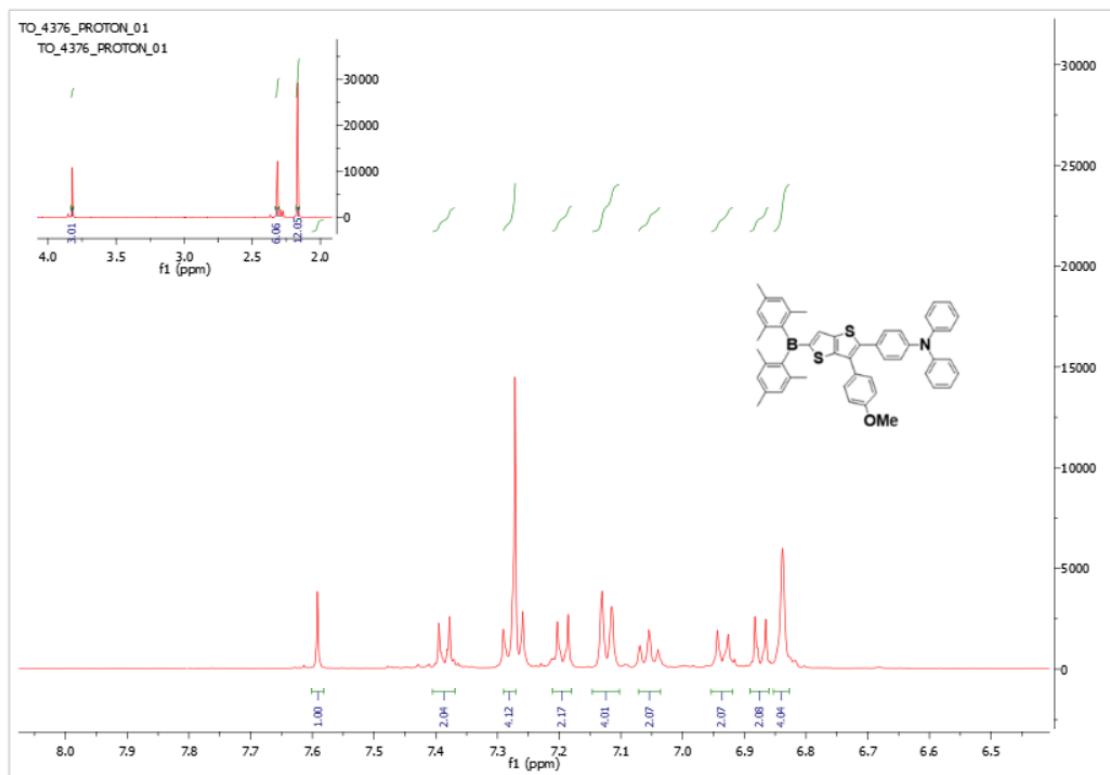
#### 4. NMR spectra



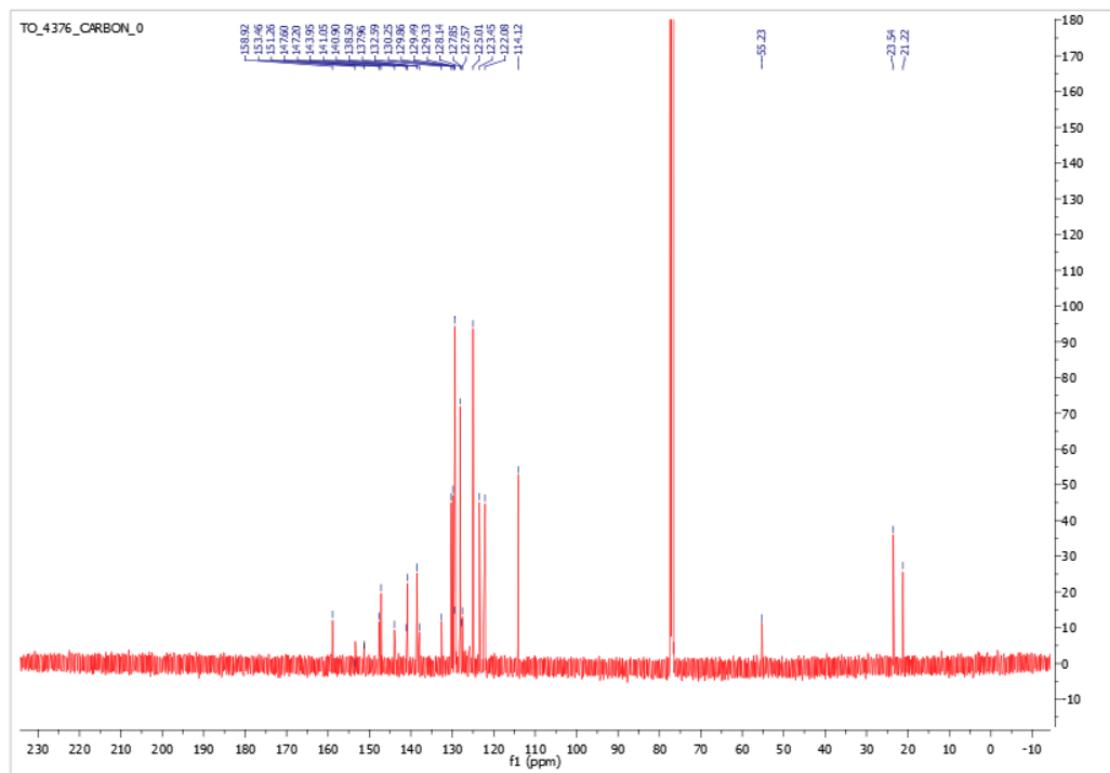
**Figure S5:**  $^1\text{H}$  NMR spectrum of 7.



**Figure S6:**  $^{13}\text{C}$  NMR spectrum of 7.



**Figure S7:**  $^1\text{H}$ -NMR spectrum of DMB-TT-TPA (**8**).



**Figure S8:**  $^{13}\text{C}$  NMR spectrum of DMB-TT-TPA (**8**).