

## **CN-Substituted *Ortho*-terphenyl Core Based High Triplet Energy Bipolar Host Materials for Stable and Efficient Blue TADF Device**

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## Supplementary information

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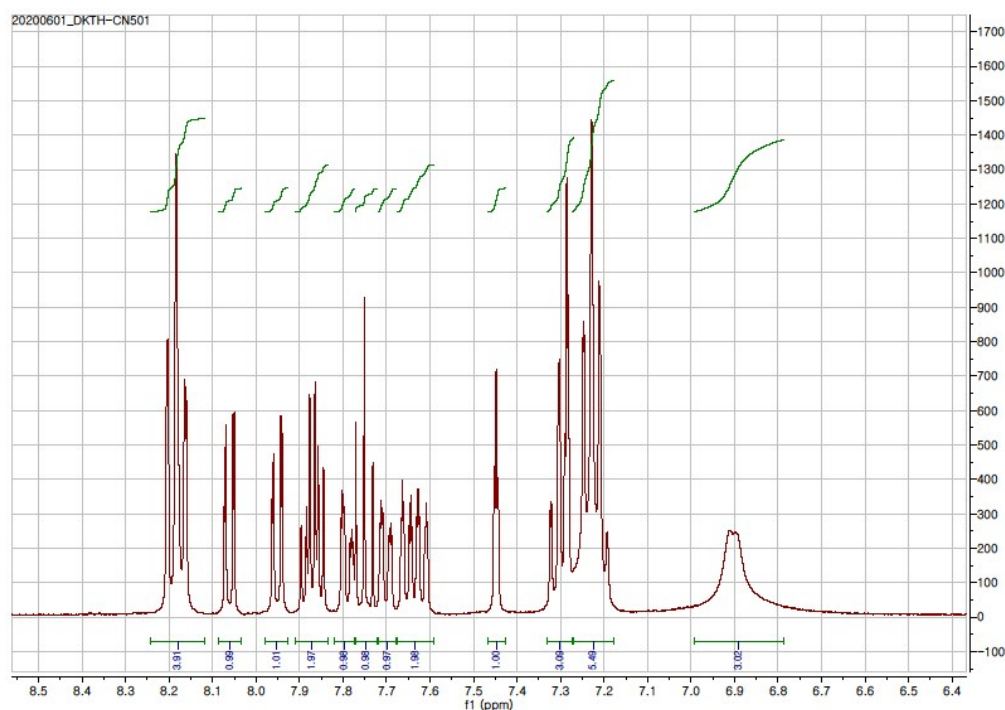
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# 1. Experimental Details

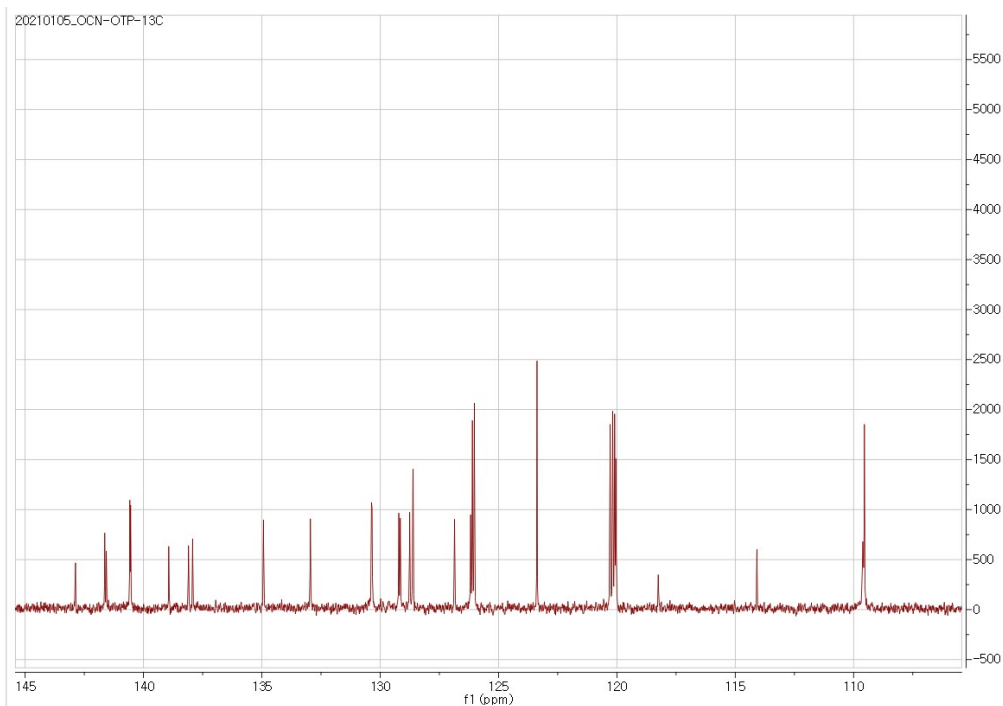
## 1.1 General information

All reagents were purchased from commercial suppliers and used as received. All solvents were used without additional purification. To verify molecular structures of the synthesized materials,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectrum was measured using Bruker Avance III-400 NMR spectrometer. High-resolution mass spectra were performed using JMS-700 (JEOL, Japan) Gas Chromatography-Mass spectrometer. The transient PL decay was measured using the Quantaurs-Tau fluorescence lifetime measurement system (C11367-03, Hamamatsu Photonics Co.) in a nitrogen-filled atmosphere.

## 2. List of figures

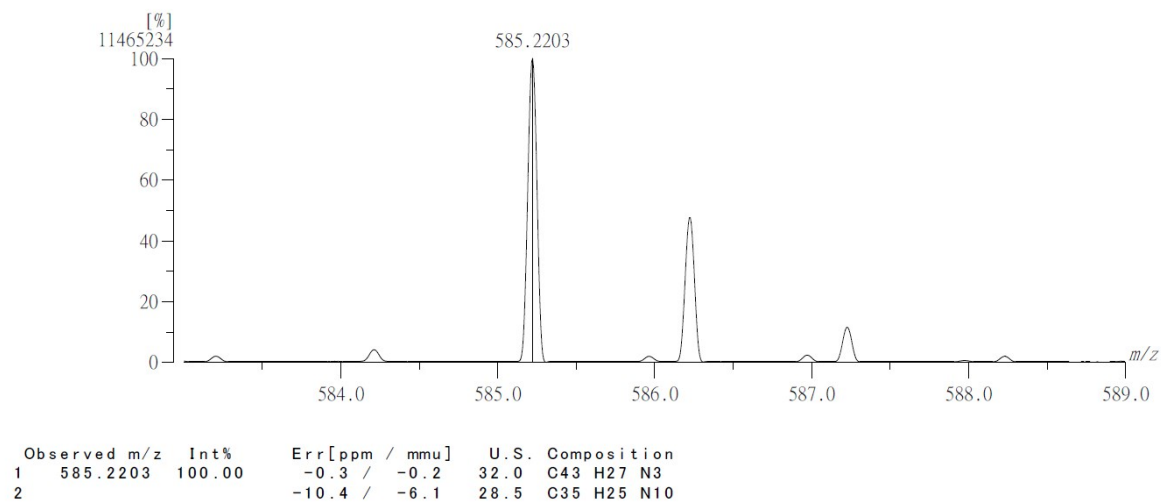


**Figure S1.**  $^1\text{H}$  NMR of *o*CN-OTP.

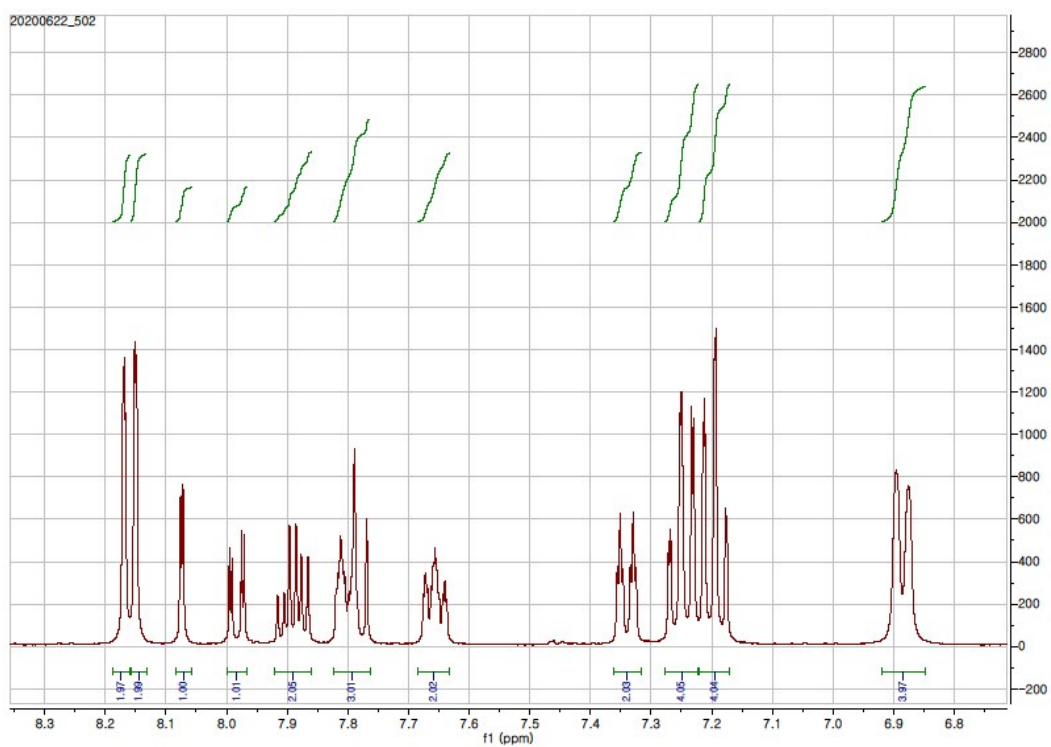


**Figure S2.**  $^{13}\text{C}$  NMR of *o*CN-OTP.

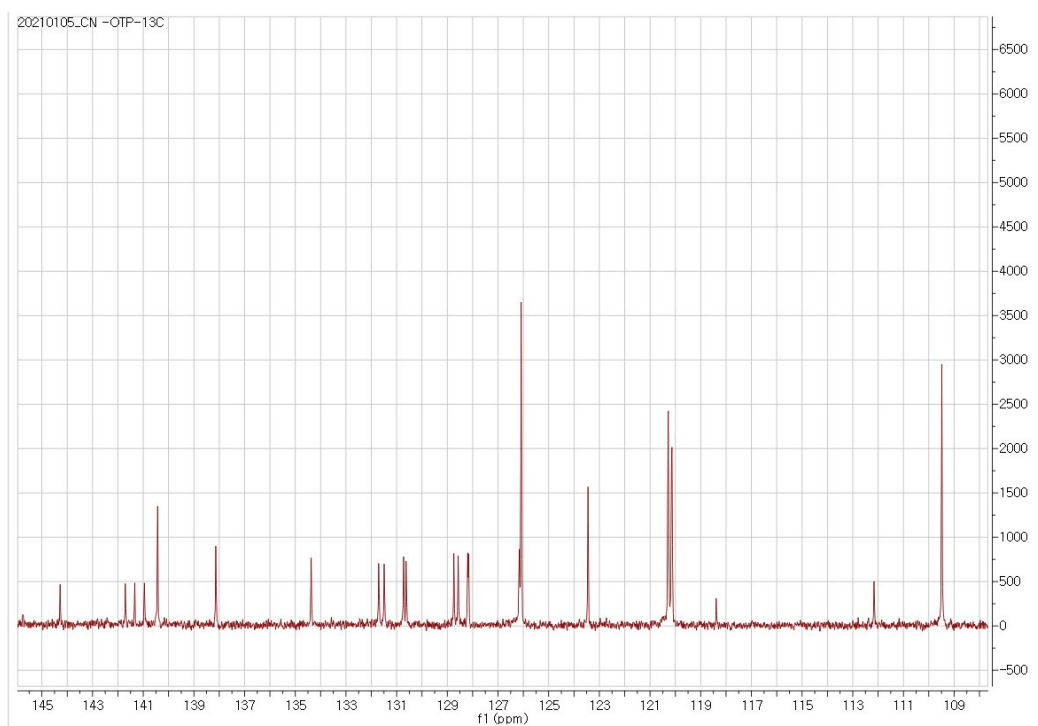
[ Mass Spectrum ]  
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 RT : 0.45 min Scan# : (14.43)  
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 Mass Tolerance : 20ppm, 5mmu if  $m/z < 250$ , 20mmu if  $m/z > 1000$   
 Unsaturation (U.S.) : -0.5 - 50.0



**Figure S3.** HRMS of *o*CN-OTP.

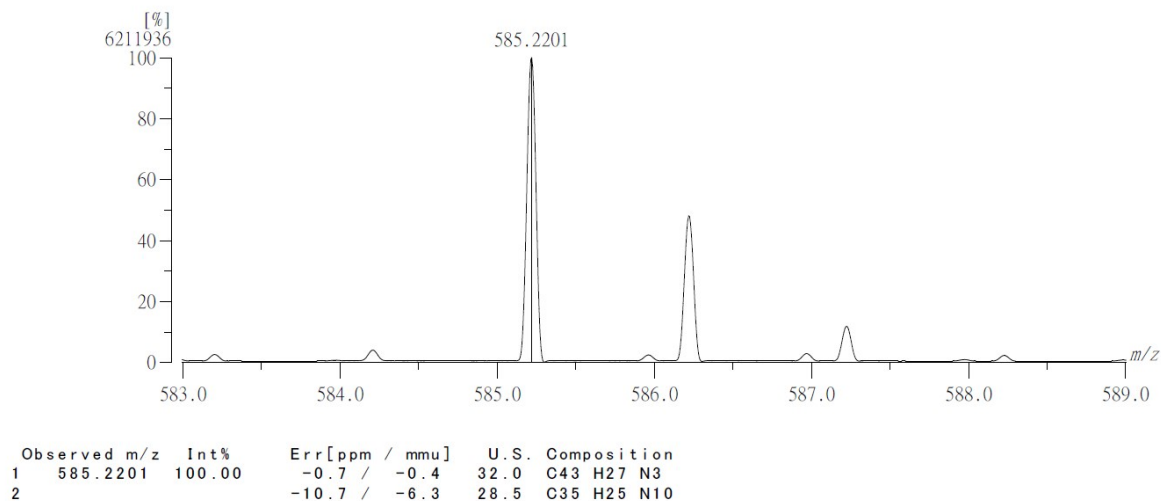


**Figure S4.**  $^1\text{H}$  NMR of *m*CN-OTP.

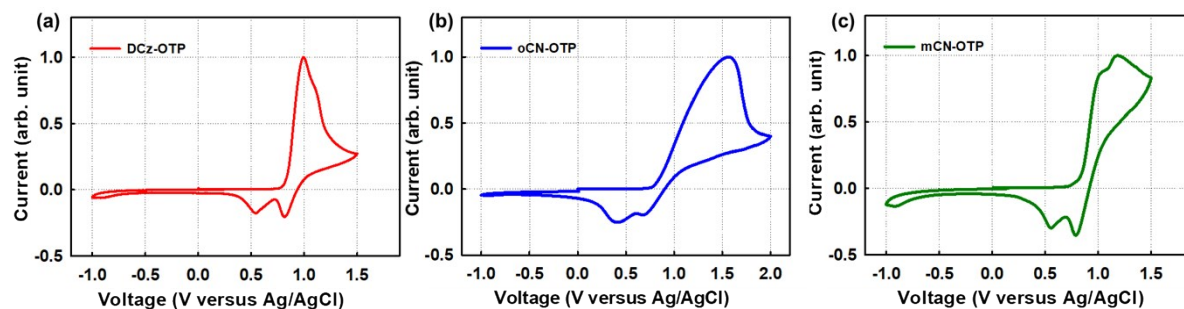


**Figure S5.**  $^{13}\text{C}$  NMR of *m*CN-OTP.

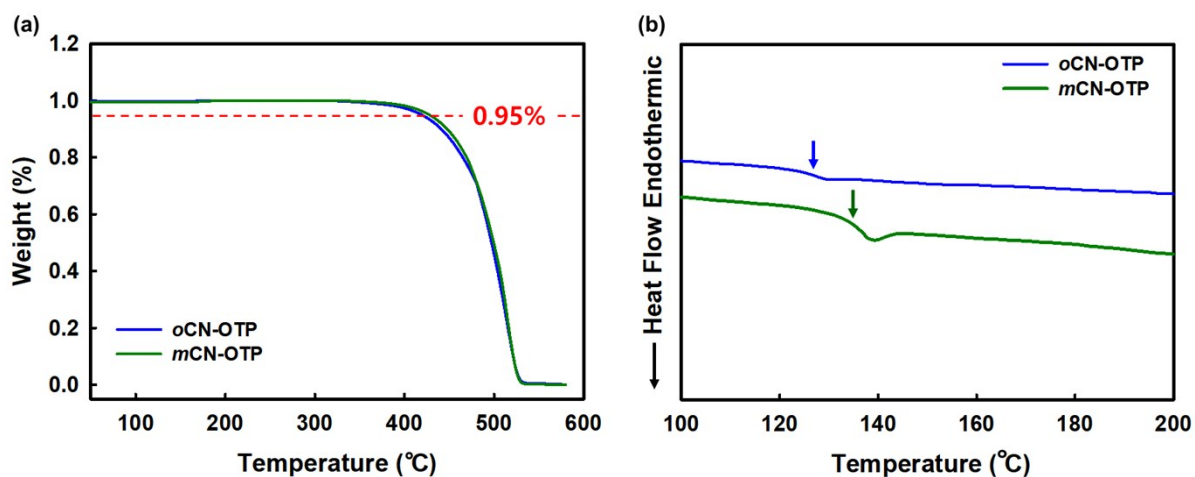
[ Mass Spectrum ]  
 Data : EI-A439 Date : 21-Jan-2021 12:08  
 RT : 1.98 min Scan# : (51,91)  
 Elements : C 100/0, H 100/0, N 10/0  
 Mass Tolerance : 20ppm, 5mmu if m/z < 250, 20mmu if m/z > 1000  
 Unsaturation (U.S.) : -0.5 - 50.0



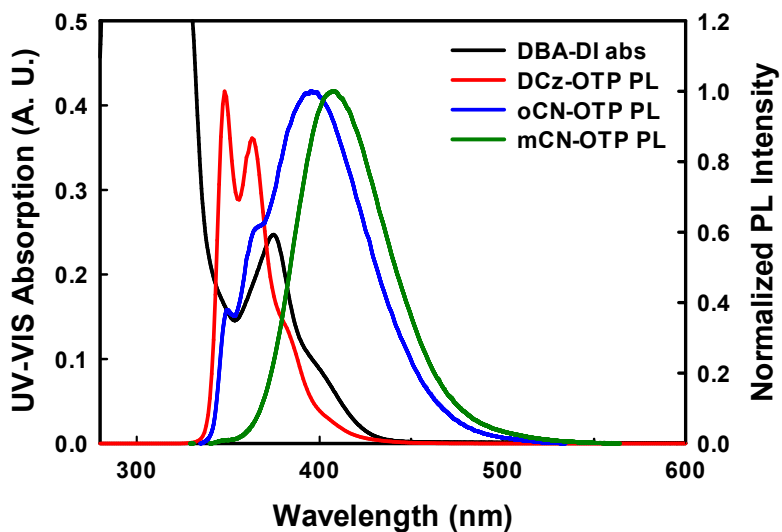
**Figure S6.** HRMS of *m*CN-OTP.



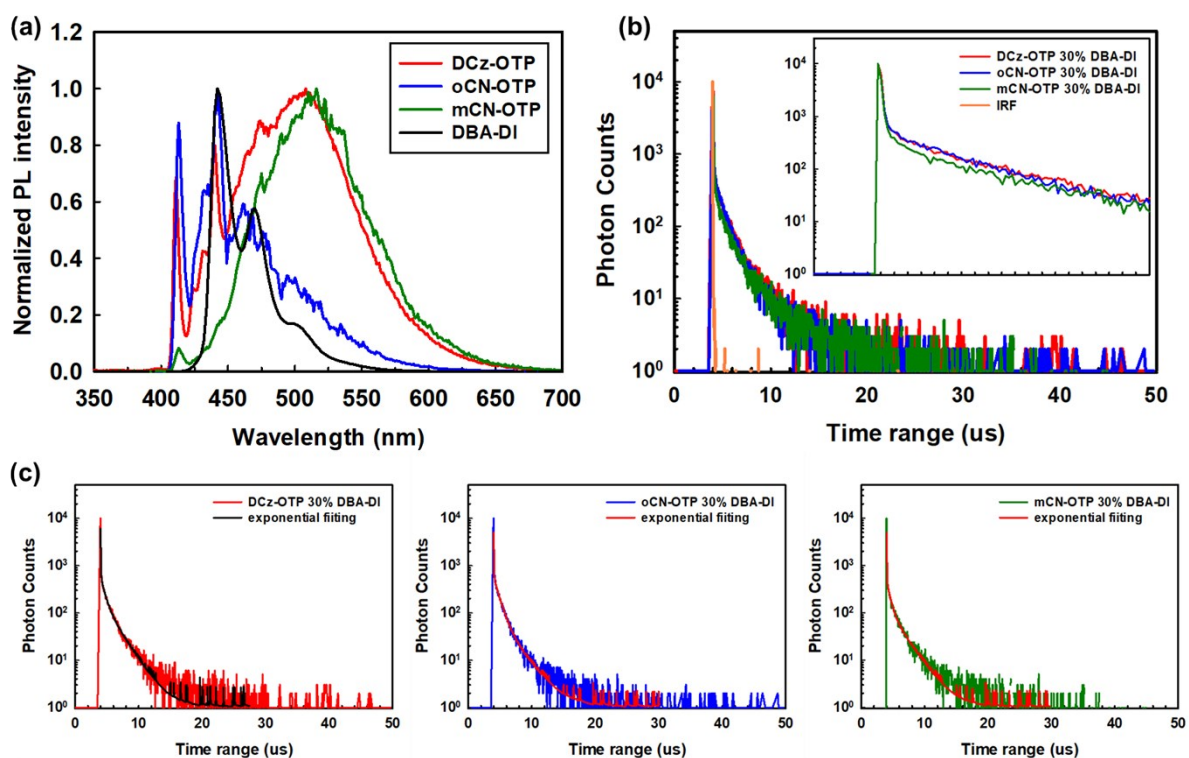
**Figure S7.** Cyclic Voltammetry (CV) cure of DCz-OTP, *o*CN-OTP and *m*CN-OTP.



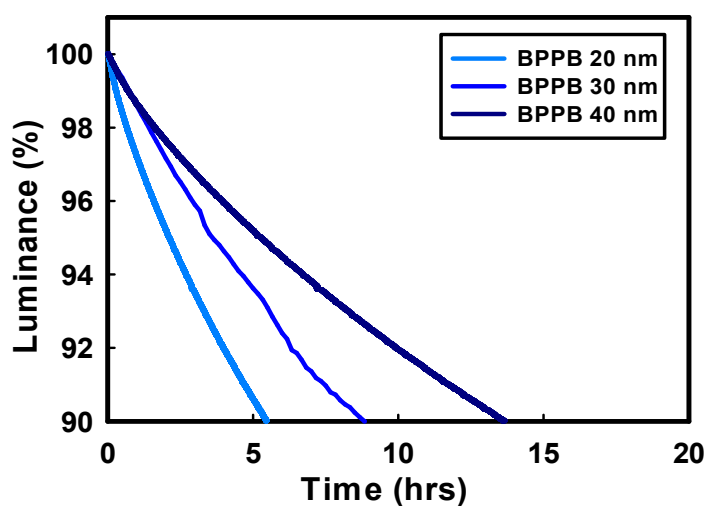
**Figure S8.** TGA and DSC graphs of DCz-OTP, *o*CN-OTP and *m*CN-OTP.



**Figure S9.** Spectral overlap between PL emission of three host and absorption of DBA-DI TADF dopant.

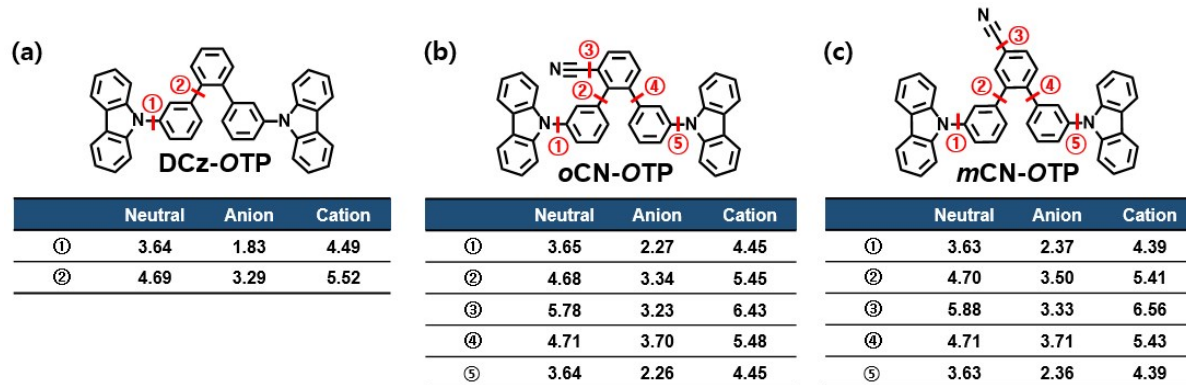


**Figure S10.** (a) Comparison of phosphorescence spectra of DCz-OTP, *o*CN-OTP, *m*CN-OTP and DBA-DI in toluene and (b) film TRPL of 30% of DBA-DI in DCz-OTP, *o*CN-OTP and *m*CN-OTP. (c) exponential fitting curve for determining decay time.



**Figure S11.** Device lifetimes of *m*CN-OTP host device depending on the thickness of BPPB at initial luminance of 1,000 cd/m<sup>2</sup>.





**Figure S12.** Calculation of Bond dissociation energies of host materials in neutral, anion, and cation states.