

Carbazole and dibenzo[b,d] furan-based hole transport materials with high thermal stability

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1. Material and apparatus

All materials and reagents were purchased from TCI, Leyan, and Bide, and immediately used without further purification. Thin-layer chromatography (TLC) was used to monitor the reaction. The chemical structure of the synthesized compounds was characterized by ^1H and ^{13}C nuclear magnetic resonance (NMR, Bruker AM 400 MHZ Avance III) in different deuterated reagents. Also, the high-resolution mass spectrometry (HRMS, Waters LCT Premier XE mass spectrometer) was used to measure compounds' molecular weight and the proportion of constituent elements was measured by elemental analysis (VARIO EL CUBE). UV-Vis absorption and fluorescence spectra were recorded on Varian Cary 500 spectrometer and Horiba spectrofluorometer (FluoroMax-4), respectively. Cyclic voltammetry was performed by a Versastat II electrochemical work station in the typical three-electrode cell with a working electrode, a reference electrode, and a counter electrode in dichloromethane solution, and 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) as the electrolyte. Furthermore, the thermal decomposition temperature (T_d), and glass transition temperature (T_g) were determined by thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC), respectively.

2. Device fabrication and measurement

Before device fabrication, the ITO glasses were washed with acetone, isopropanol, and distilled water in the ultrasound system. Then, the ITO glasses were activated by ozone for 10 minutes. All chemical materials were evaporated under pressure of 10^{-5} Pa, and the deposition rate was controlled in the range of 0.1 to 3 \AA s^{-1} . At last, the devices were measured by Keithley 2400 source meter and Minolta CS-2000 spectrometer to obtain the electroluminescent properties at room temperature in a dark environment.

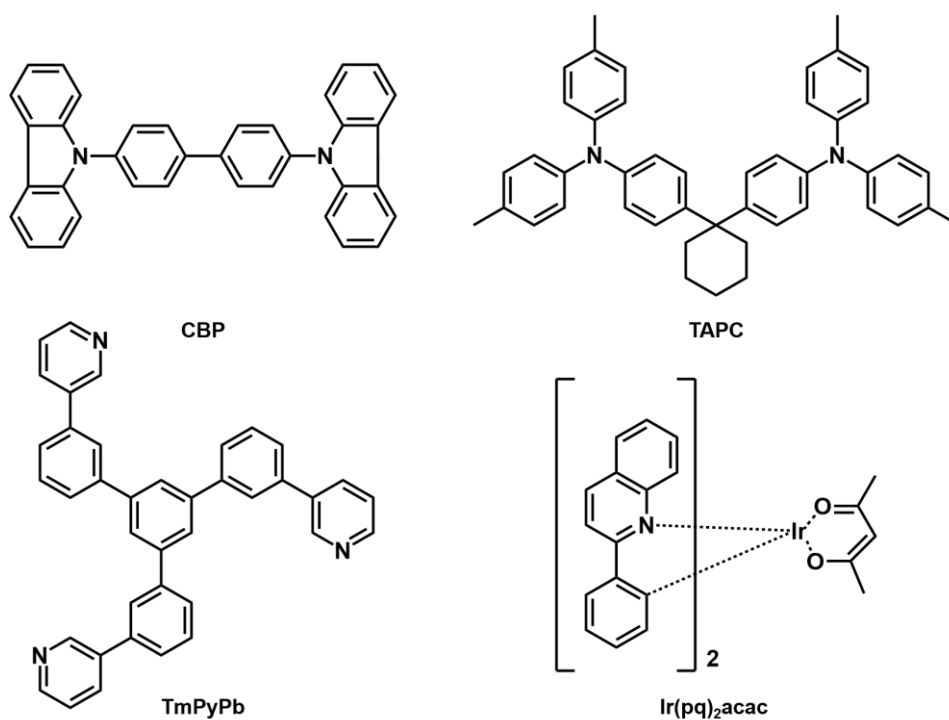


Figure S1. Compounds involved in devices.

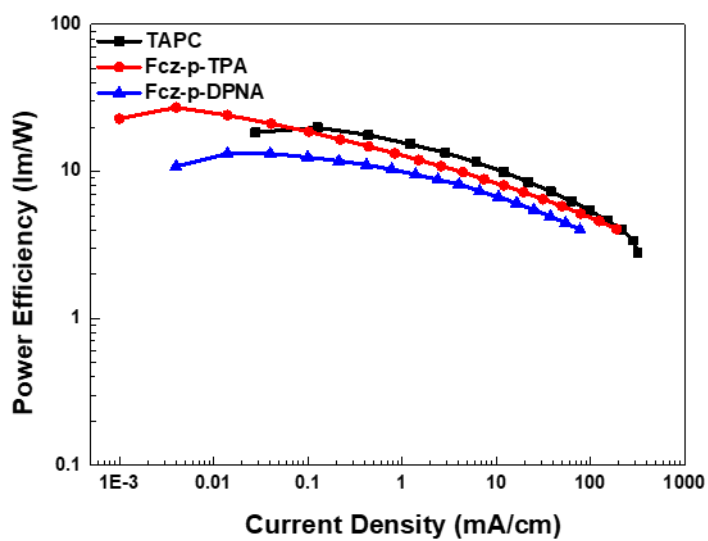
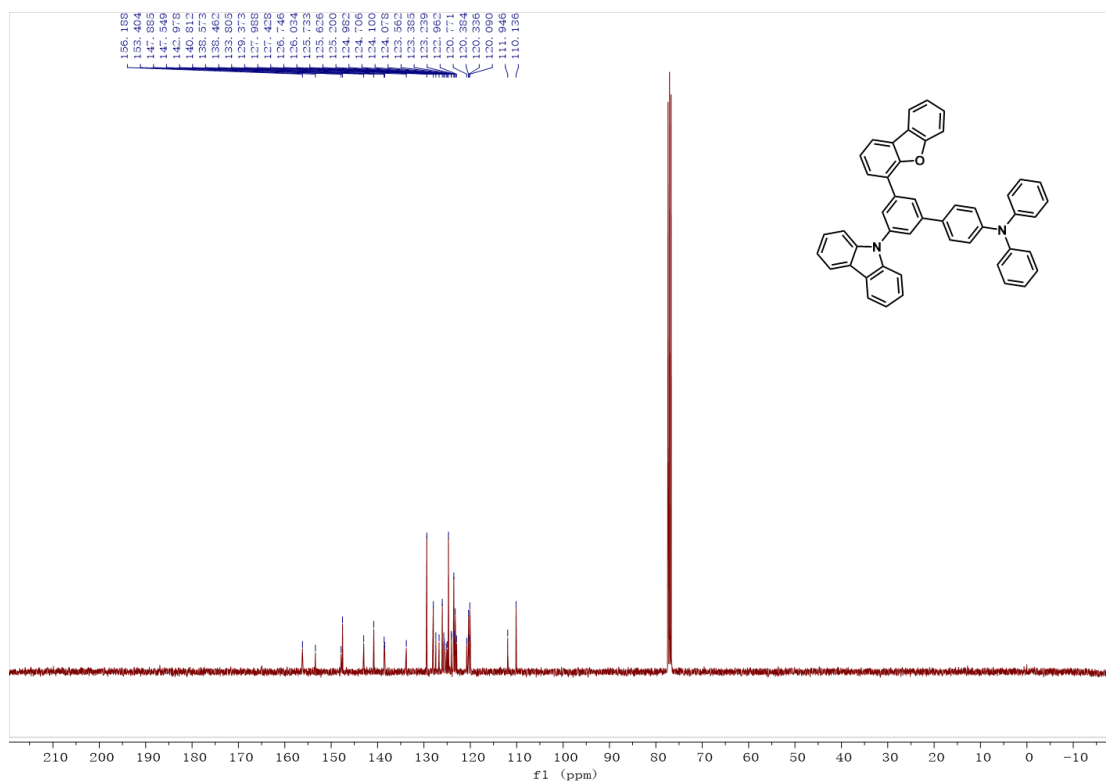


Figure S2. Power efficiency-Current density (PE-CD) curve of devices.

Table S1. Roll-off of EQE based on current density.

Compound	1-10 mA cm ⁻²	1-100 mA cm ⁻²	10-100 mA cm ⁻²
FCzTPA	11.4%	33.9%	24.4%
FCzDPNA	12.5%	38.7%	29.9%
TAPC	14.8%	41.7%	31.5%



¹³C NMR of FCzTPA in CDCl₃.

Elemental Composition Report

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Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

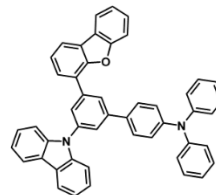
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

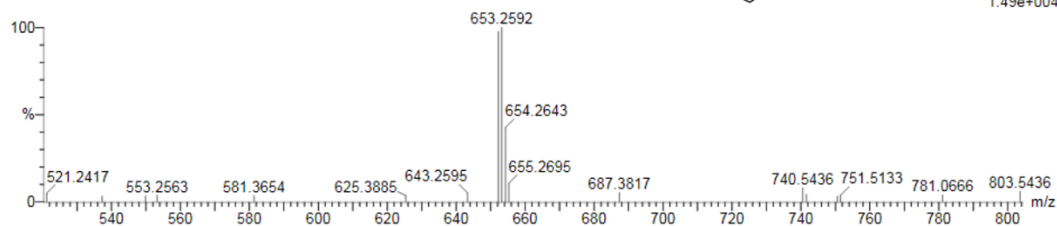
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H-TIAN

TH-SJ-06 49 (0.543) Cm (46:49)



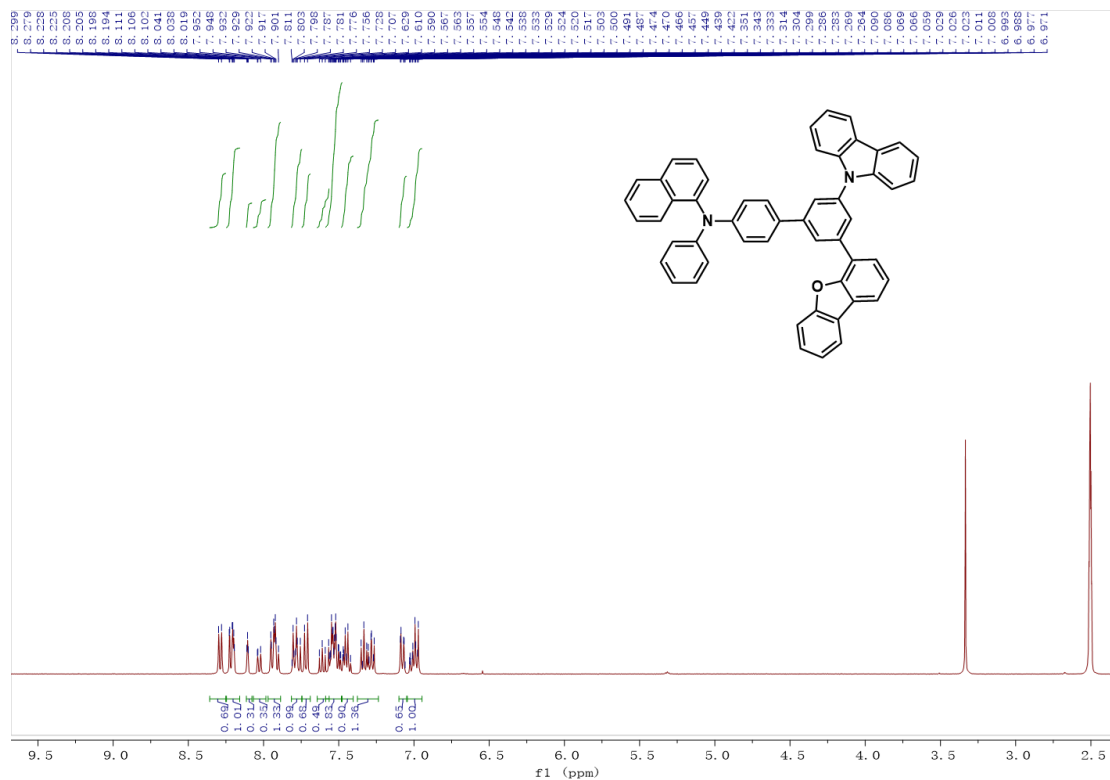
1: TOF MS ES+
1.49e+004



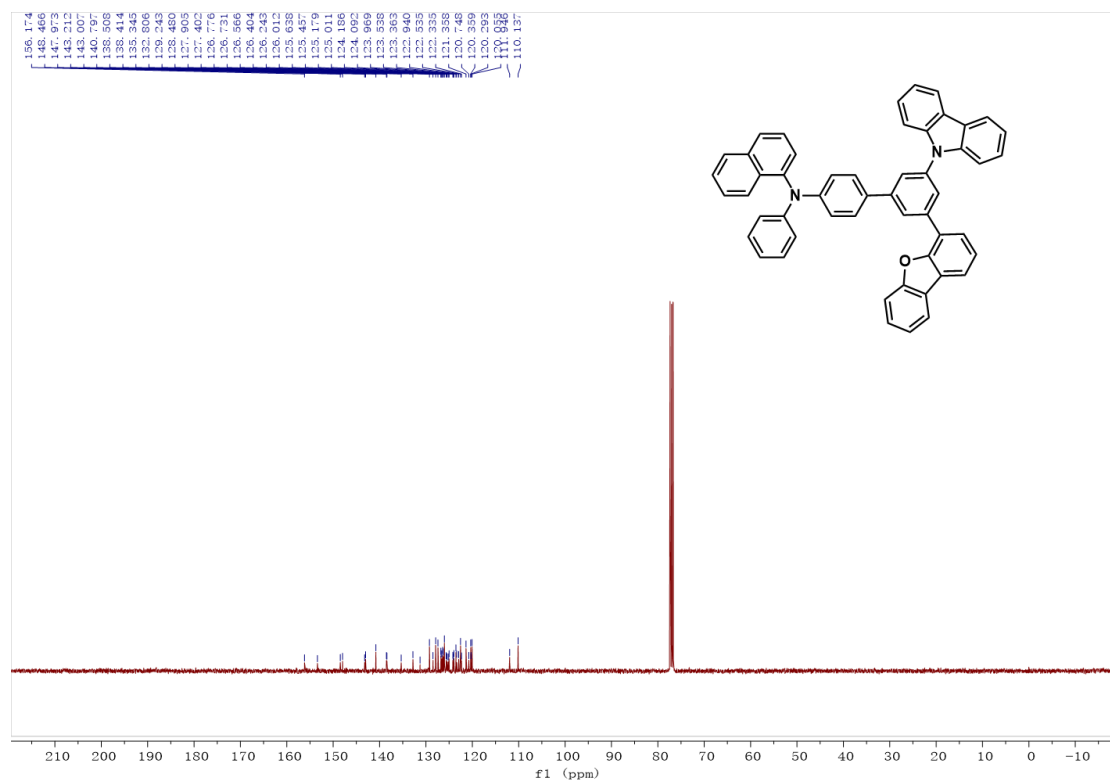
Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
653.2592	653.2593	-0.1	-0.2	33.5	16.9	0.0	C ₄₈ H ₃₃ N ₂ O

HRMS of FCzTPA in DCM.



¹H NMR of FCzDPNA in DMSO-*d*₆.



¹³C NMR of FCzDPNA in CDCl₃.

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

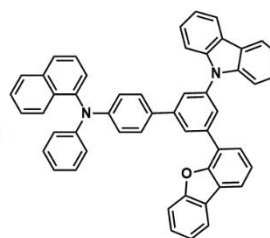
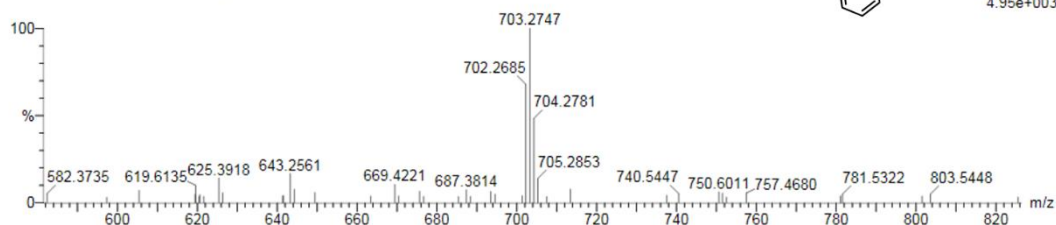
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-52 H: 0-35 N: 0-2 O: 0-1

H-TIAN

TH-SJ-07 34 (0.380) Cm (33:37)

1: TOF MS ES+
4.95e+003

Minimum: -1.5
Maximum: 5.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
703.2747	703.2749	-0.2	-0.3	36.5	13.0	0.0	C52 H35 N2 O

HRMS of FCzDPNA in DCM.