Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary information

Systematic Investigation *via* Controlling the Energy Gap of Local and Charge-Transfer Triplet State for Enabling High Efficiency Thermally Activated Delayed Fluorescence Emitter

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1. Materials and Methods

1.1. Chemicals

All chemicals were used as received unless otherwise stated. The chemicals were received from Sigma-Aldrich, Merck India, and Alfa aesar.

1.2. Instrumentation

The ^{1}H and ^{13}C NMR spectra were recorded by using Bruker Avance 400 spectrometer. The HRMS were measured using MAT-95XL HRMS or MStation. The ultraviolet-visible (UV) absorption spectra were taken using PerkinElmer Lambda 750 UV-VIS spectrophotometer. Fluorescence and phosphorescence spectra were recorded on a Hitachi F-7100 spectrophotometer. The absolute PL quantum efficiency of the doped films were determined using an integrating sphere under N_2 atmosphere. The time-resolved emission spectra and decays of doped films were recorded using an Edinburgh Instruments FLS980 spectrometer equipped with a double monochromator for both excitation and emission, operating in right-angle geometry mode and the highly sensitive photomultiplier tube (RED PMT in Cooled Housing) positioned after a double emission monochromator.

The thermal stability of these four materials was studied using TA Instruments Q50 TGA thermogravimetric analyzer. The TGA curve was recorded under N_2 flow from room temperature to 600 °C. The cyclic voltammetry measurement was carried out in deoxygenated dichloromethane (DCM) with 0.1 M tetrabutylammonium hexafluorophosphate (TBAP) as supporting electrolyte in a three-electrode system using BioLogic SP300 potentiostat (BioLogic, France). Glassy Carbon, Platinum wire (Pt) and Ag/AgCl/KCl(saturated) were used as working, counter and reference electrodes, respectively. The scan rate was kept at 100 mV/s for the measurement. The HOMO energy levels were determined from the onset of the oxidation potential using the equation $-(4.8\text{ eV} + E_{ox}\text{ (vs }Fc_{ox}))$ while the LUMO energy levels were calculated from optical Band gap (E_g) and the HOMO levels.

1.3. OLEDs Fabrication and Measurement

Emitting materials used in device fabrication were purified by vacuum sublimation. Other materials such as NPB, TAPC, DPEPO, mCBP, CBP, PPT, and TmPyPb were purchased from the commercial source (Lumtec) and used without further purification. The devices were fabricated by vacuum deposition onto pre-coated ITO glass with sheet resistance of 15 Ω/square at a pressure lower than 10^{-6} Torr. The organic materials were deposited at the rate of 0.5~1.2 Å s^{-1}. LiF and Al were deposited at the rate of 0.1 Å s^{-1}, 3-10 Å s^{-1} respectively. The rest of the procedures are similar to the reported method.[1,2]

The transient electroluminescence measurements were carried out on a function generator (Agilent 8114A) and an indigenously developed time-resolved emission spectrometer. The devices were driven by a voltage pulse of 6 V with a repetition rate of 20 kHz and pulse width of 10 μs. The emission decay curves at specific wavelengths were gained using a cooled photomultiplier tube (PMT) detector (Becker & Hickl GmbH PMC-100) integrated with a 300 nm focal length monochromator (Princeton Instruments Acton SP2300). The time-resolved photon counting was done via a multichannel scaling (MCS) card (Becker & Hickl GmbH MSA-300) with a time resolution of 5 ns. The whole system was synchronized with a digital delay generator (Stanford Research Systems DG645).

2. Synthesis of targeted compounds

Synthesis of (3,5-dibromophenyl)(pyridin-3-yl) methanone (3BPy)[3]

In a flame dried two neck flask under nitrogen atmosphere 1,3,5-tribromobenzene (5 g, 15.88 mmol) was dissolved in 160 mL of diethyl ether, and the solution was cooled to –78 °C using acetone and liquid nitrogen composition. A solution of *n*-BuLi (1.6 M in hexane, 11.66 mL, 17.47 mmol) was added dropwise at -78 °C. The reaction mixture was stirred for 30 min at -78 °C, and a solution of 3-cyanopyridine (1.65 g, 15.88 mmol) in diethyl ether (20 mL) was added slowly. The mixture was stirred at -78 °C for 1 h and slowly allowed to warm to 25 °C, then 2 N HCl (50 mL) was added and the mixture was stirred for 2 h at room temperature. The mixture was made basic by the addition of 1 N NaOH. The product was extracted with EtOAc (2 x 150 ml) and the combined organic layers were dried over Na_2SO_4 filtered, concentrated in *vacuo* and the crude product was purified by a silica gel column chromatography using ethyl acetate/n-hexane as the eluent to afford (3,5-dibromophenyl)(pyridin-3-yl)methanone (3BPy) as white crystalline solid. (4.2 g, 77% yield); $R_f = 0.47$ (3:7 EtOAc : hexane, silica gel); **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.96 (dd, $J = 2.29, 0.92$ Hz, 1H), 8.84 (dd, $J = 4.86, 1.71$ Hz, 1H), 8.09 (ddd, $J = 7.93, 2.27, 1.71$ Hz, 1H), 7.91 (t, $J = 1.76$ Hz, 1H), 7.83 (d, $J = 1.75$ Hz, 2H), 7.48(ddd, $J = 7.94, 4.86, 0.91$ Hz, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$): δ 192.19, 153.82, 151.05, 139.85, 138.54, 137.35, 131.64, 123.88, 123.67 ppm; **HRMS (ESI-TOF)** m/z: $[M]^+$ Calculated for $C_{12}H_7Br_2NO$ 338.8894; Found 338.8890.

Synthesis of (3,5-di(9*H*-carbazol-9-yl)phenyl)(pyridin-3-yl)methanone (3BPy-*m*DCz)[2]

3,5-di(9*H*-carbazol-9-yl)phenyl)(pyridin-3-yl)methanone (3BPy-*m*DCz) was synthesized using a reported literature.[2] To an oven-dried seal tube initially fitted with a septum were added (3,5-dibromophenyl)(pyridin-3-yl) methanone (3BPy) (3.0 g, 8.8 mmol), carbazole (3.68 g, 21.9 mmol), Cu (1.12 g, 17.6 mmol), K_2CO_3 (6.08 g, 43.98 mmol) and 1,2-dichlorobenzene (20 mL). The tube was evacuated and purged with nitrogen three times. Then, the septum was removed and the sealed tube was locked with a screw cap under nitrogen atmosphere. The suspension was stirred at 180 °C for 48 h. After completion of the reaction, the reaction mixture was diluted with ethyl acetate (30 mL), filtered through combination of Celite and Silica pad, and washed with ethyl acetate (3 X 30 mL). The combined filtrate was concentrated under reduced pressure and the residue was purified by a silica gel column chromatography using ethyl acetate/*n*-hexane as the eluent to afford (3,5-di(9*H*-carbazol-9-yl)phenyl)(pyridin-3-yl)methanone (3BPy-*m*DCz) as a weightless light yellow solid. (2.66 g, 59% yield); $R_f = 0.40$ (3:7 EtOAc : hexane, silica gel); **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.19 (dd, J = 2.32, 0.89 Hz, 1H), 8.84 (dd, $J = 4.86, 1.74$ Hz, 1H), 8.26 (dt, $J = 7.93, 1.97, 1.97$ Hz, 1H), 8.16 (d, $J = 7.81$

Hz, 3H), 8.13 (s , 3H), 7.57 (d, J = 8.29, 3H), 7.48 (ddd, *J* = 8.27, 7.12, 1.24 Hz, 6H), 7.34 (ddd, *J* = 7.96, 7.12, 0.97 Hz, 5H); ^{13}**C NMR** (126 MHz, $CDCl_3$): *δ* 193.63, 150.85, 143.42, 140.33, 140.23, 139.43, 129.68, 126.69, 126.56, 123.99, 122.82, 121.05, 120.81, 109.46 ppm; **HRMS (ESI-TOF)** m/z*:* $[M]^+$ Calculated for $C_{36}H_{24}N_3O$ 513.1841; Found 513.1822.

Synthesis of (3,5-bis(di-*p*-tolylamino)phenyl)(pyridine-3-yl)methanone (3BPy-*m*DTA).

To an oven-dried seal tube initially fitted with a septum were added (3,5-dibromophenyl)(pyridine-3-yl) methanone (3BPy) (1.00 g, 2.93 mmol), Di-*p*-tolylamine (1.16 g, 5.87 mmol) , $Pd_2(dba)_3$ (0.10 g, 0.10 mmol), Sodium *tert*-butoxide (1.40 g, 14.66 mmol) , *t*-Bu_3PHBF_4 (0.26 g, 0.88 mmol) and dry toluene (20 mL). The tube was evacuated and purged with nitrogen three times. Then, the septum was removed and the seal tube was locked with screw cap under nitrogen atmosphere. The suspension was stirred at 125 °C for 48 h. After completion of reaction, the reaction mixture was diluted with ethyl acetate (30 mL), filtered through combination of Celite and Silica bed, and washed with ethyl acetate (3 X 30 mL). The combined filtrate was concentrated under reduced pressure and the residue was purified by a silica gel column chromatography using ethyl acetate/*n*-hexane as eluent to afford 3BPy-*m*DTA as a yellowish-orange crystalline solid (0.95 g, 56% yield); R_f = 0.48 (3:7 EtOAc : hexane, Silica gel); ^{1}**H NMR** (500 MHz, $CDCl_3$): δ 8.95 (d, *J* = 2.35 Hz, 1H), 8.71 (dd, *J* = 4.85,1.74 Hz, 1H), 8.02 (dt, *J* = 7.91, 1.97, 1.97 Hz, 1H), 7.31 (ddd, *J* = 7.92, 4.85, 0.91 Hz, 1H), 7.04 (m, 8H), 6.99 (d, *J* = 8.55 Hz, 8H), 6.92 (t, *J* = 2.13, 2.13 Hz, 1H), 6.89 (d, *J* = 2.12 Hz, 2H), 2.29 (s,12H) ppm; ^{13}**C NMR** (126 MHz, $CDCl_3$) : δ 194.92, 152.99, 151.31, 149.36, 144.75, 138.52, 137.45, 133.19, 130.18, 124.87, 123.28, 120.03, 116.29, 21.05 ppm ; **HRMS (ESI-TOF)** m/z : $[M]^+$ Calculated for $C_{40}H_{35}N_3O$ 573.2780 ; Found 573.2774.

Synthesis of (3,5-bis(9,9-dimethylacridin-10(9*H*)-yl)phenyl(pyridin-3-yl)methanone (3BPy-*m*DMAC).

To an oven-dried seal tube initially fitted with a septum were added (3,5-dibromophenyl)(pyridine-3-yl) methanone (3BPy) (1.00 g, 2.93 mmol), 9,9-dimethyl-9,10-dihydroacridine (1.22 g, 5.87 mmol) , $Pd_2(dba)_3$ (0.1 g, 0.10 mmol), Sodium *tert*-butoxide (1.40 g, 14.66 mmol) , *t*-Bu_3PHBF_4 (0.26 g, 0.88 mmol) and dry toluene (20 mL). The tube was evacuated and purged with nitrogen three times. Then, the septum was removed and the seal tube was locked with screw cap under nitrogen atmosphere. The suspension was stirred at 125 ℃ for 48 h. After completion of reaction, the reaction mixture was diluted with ethyl acetate (30 mL), filtered through combination of Celite and Silica bed, and washed with ethyl acetate (3 X 30 mL). The combined filtrate was concentrated under reduced pressure and the residue was purified by a silica gel column chromatography using ethyl acetate/*n*-hexane as eluent to afford 3BPy-*m*DMAC as a yellow crystalline solid (0.92 g, 52% yield); $R_f = 0.54$ (3:7 EtOAc : hexane, Silica gel); **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.11 (dd, *J* = 2.28, 0.90 Hz, 1H), 8.81 (dd, *J* = 4.85, 1.75 Hz, 1H), 8.20 (dt, *J* = 7.89, 1.96, 1.96 Hz, 1H), 8.01 (d, *J* = 1.96 Hz, 2H), 7.69 (t, *J* = 1.92, 1.92 Hz, 1H), 7.47 (m, 5H), 7.08 (ddd, *J* = 8.28, 7.30, 1.57 Hz, 4H), 6.98 (td, *J* = 7.53, 7.53, 1.27 Hz, 4H), 6.43 (dd, *J* = 8.23, 1.28 Hz, 4H), 1.67 (s, 12H) ppm; **^{13}C NMR** (126 MHz, $CDCl_3$) : δ 192.77, 153.30, 150.71, 144.62, 141.76, 140.28, 139.89, 137.11, 132.87, 132.39, 130.52, 126.59, 125.57, 123.63, 121.32, 113.83, 35.99, 31.13 ppm; **HRMS (ESI-TOF)** m/z : $[M]^+$ Calculated for $C_{42}H_{35}N_3O$ 597.2780 ; Found 597.2758.

Synthesis of (3,5-di(10H-phenothiazin-10-yl)phenyl)(pyridin-3-yl)methanone (3BPy-*m*DPT).

To an oven-dried seal tube initially fitted with a septum were added (3,5-dibromophenyl)(pyridine-3-yl) methanone (3BPy) (1.00 g, 2.93 mmol), 10*H*-phenothiazine (1.17 g, 5.87 mmol) , $Pd_2(dba)_3$ (0.1 g, 0.10 mmol) , Sodium *tert*-butoxide (1.40 g, 14.66 mmol) , *t*-Bu_3PHBF_4 (0.26 g, 0.88 mmol) and dry toluene (20 mL). The tube was evacuated and purged with Nitrogen three times. Then, the septum was removed and the seal tube was locked with screw cap under nitrogen atmosphere. The suspension was stirred at 125℃ for 48 h. After completion of reaction, the reaction mixture was diluted with ethyl acetate (30 mL), filtered through combination of Celite and Silica bed, and washed with ethyl acetate (3 X 30 mL). The combined filtrate was concentrated under reduced pressure and the residue was purified by a silica gel column chromatography using ethyl acetate/*n*-hexane as eluent to afford 3BPy-*m*DPT as an orange crystalline solid (0.80 g, 47% yield); R_f = 0.32 (3:7 EtOAc : hexane, Silica gel); **^{1}H NMR** (500 MHz,$CDCl_3$) : δ 9.00 (d, *J* = 2.01 Hz, 1H), 8.77 (dd, *J* = 4.85, 1.71 Hz, 1H), 8.10 (dt, *J* = 7.91, 1.99, 1.99 Hz, 1H), 7.57 (dd, *J* =2.14, 1.06 Hz, 2H), 7.40 (m, 2H), 7.20 (dd, *J* = 7.68, 1.55 Hz, 4H), 7.08 (td, *J* = 7.94, 7.74, 1.57 Hz, 4H) , 6.99 (td, *J* = 7.52, 7.45, 1.28 Hz, 4H), 6.76 (dd, *J* = 8.06, 1.24 Hz, 4H) ppm; **^{13}C NMR** (126 MHz, $CDCl_3$): δ 193.52, 152.98, 150.67, 145.45, 142.77, 140.15, 137.40, 132.79, 127.96, 127.39, 126.31, 125.28, 124.51, 123.62, 122.60, 120.49 ppm; **HRMS (ESI-TOF)** m/z : $[M\ ]^+$ Calculated for $C_{36}H_{23}N_3OS_2$ 577.1282; Found 577.1287

3. Thermal Stability

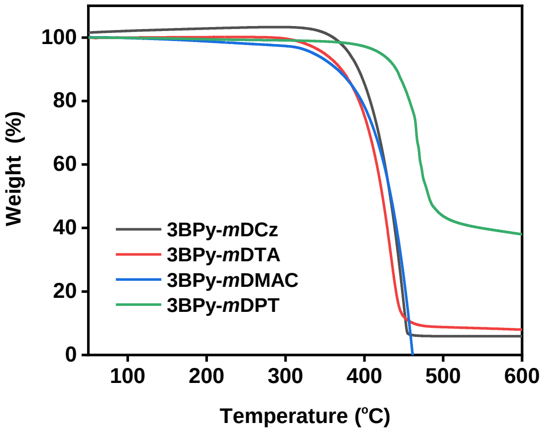


Figure S1: Thermogravimetric analysis (TGA) of 3BPy-*m*DCz, 3BPy-*m*DTA, 3BPy-*m*DMAC and 3BPy-*m*DPT under N_2 atmosphere

4. Theoretical Investigations

A time-dependent density functional theory (TDDFT, spin unrestricted) investigation for all the Donor-Acceptor emitters were performed using the Gaussian 09 program package in the delta-cluster of **SERC facility @ IISc**. The ground state molecular geometries of Donor-Acceptor emitters were optimized employing density functional theory (DFT) B3LYP hybrid functional and 6-31G (d,p) basis set in Gaussian 09 Revision A.02 software.[4,5] The TDDFT calculations with the same functionality and the basis set were employed to obtain the excited-state structure. GaussView 5.0 and Chemcraft (version 1.8) were used to analyze the molecular orbitals. The iso values ±0.03 and ±0.001 were used for the HOMO-LUMO orbital picture and hole-electron distributions respectively.

Table S1: Summary of the computational and experimental outcome: Energy of first singlet state (S_1), oscillator strength (*f*), energy of first triplet state (T_1) and energy gap between S_1 and T_1 (ΔE_{ST}) were calculated using DFT at the B3LYP/6-3111g (d,p) level in vacuum; overlap integral between hole and electron were calculated using *Multiwfn*.[6]

Compound	Donor	HOMO/LUMO/E_g (eV)	S_1 (eV)	*f*	T_1 (eV)	ΔE_{ST}# (eV)
3BPy-*m*DCz	Carbazole	-5.84/-2.16/ 3.68	3.01	0.026	2.82	0.19
3BPy-*m*DTA	Ditolylamine	-5.09/-1.62/3.47	2.80	0.039	2.56	0.24
3BPy-*m*DMAC	Dimethylacridine	-5.30/-2.12/3.18	2.50	0.004	2.47	0.03
3BPy-*m*DPT	Phenothiazine	-5.41/-2.23/3.18	2.52	0.001	2.50	0.02

#*Theoretical results*

5. Electrochemical Measurement

Electrochemical measurements were performed in 0.1 M NBu_4PF_6 (99%, Sigma Aldrich, dried) in dichloromethane (CHROMASOLV®, 99.9% Sigma Aldrich). Solutions were purged with argon prior to measurement. Electrodes: Working (Glassy Carbon - 1 mm of diameter), Counter (Pt wire) and Reference (Ag/AgCl/saturated/KCl) calibrated against ferrocene.

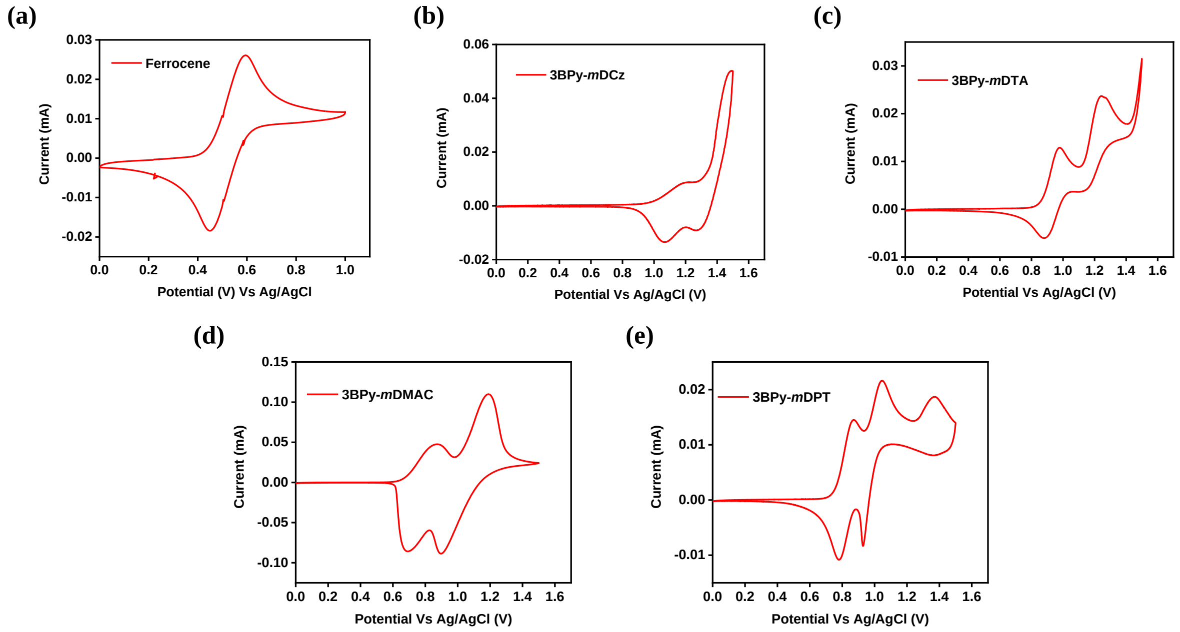


Figure S2: (a) Cyclic voltammogram (100 mV/s) of Ferrocene; (b) – (e) oxidation potential curve of 3BPy-*m*DCz, 3BPy-*m*DTA, 3BPy-*m*DMAC and 3BPy-*m*DPT respectively in de-aerated DCM (1 mM solution) using 0.1 M tetrabutylammonium hexafluorophosphate (TBAP) as supporting electrolyte, Glassy Carbon as the working electrode and Ag/AgCl/saturated KCl as a reference electrode. The HOMO values are calculated from the observed oxidation potential and the corresponding LUMO values are calculated from the following formula: $E_{LUMO} = E_{HOMO} - E_g$ where E_g is the optical band gap calculated from the absorption spectrum.

Table S2: Summary of Electrochemical Measurement

Compound	Eg (eV)	HOMO (eV)	LUMO (eV)
3BPy-*m*DCz	3.00	-5.26	-2.26
3BPy-*m*DTA	2.60	-5.14	-2.54
3BPy-*m*DMAC	2.70	-4.95	-2.25
3BPy-*m*DPT	2.38	-5.03	-2.65

6. Absorbance Study

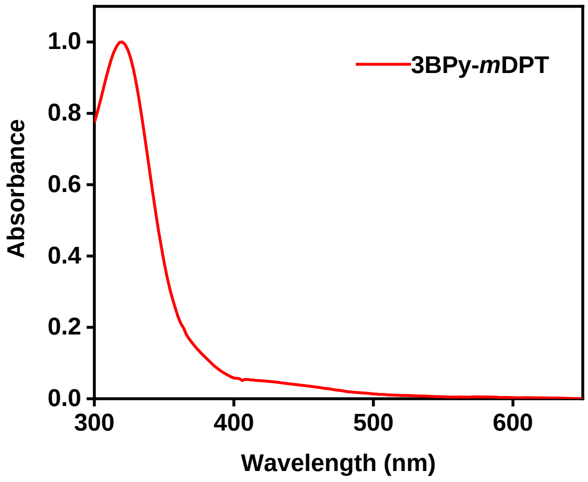


Figure S3: Absorbance spectra of 3BPy-*m*DPT in 10 µM toluene solution

7. Solvatochromic Study

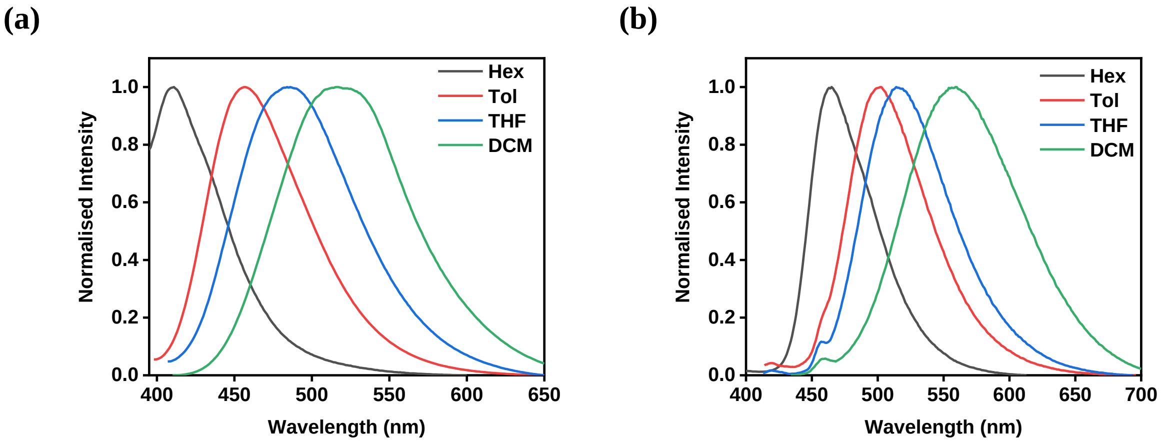


Figure S4: Emission spectra of (a) 3BPy-*m*DCz and (b) 3BPy-*m*DTA in various solvents (10µM) at 298 K.

8. Temperature dependent Transient PL

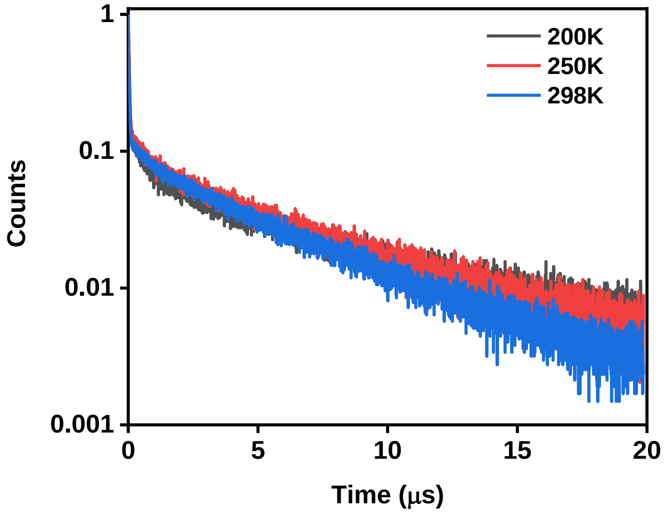


Figure S5: Temperature dependent transient PL of 7 wt% 3BPy-*m*DMAC: *m*CBP doped film

9. Device Architecture

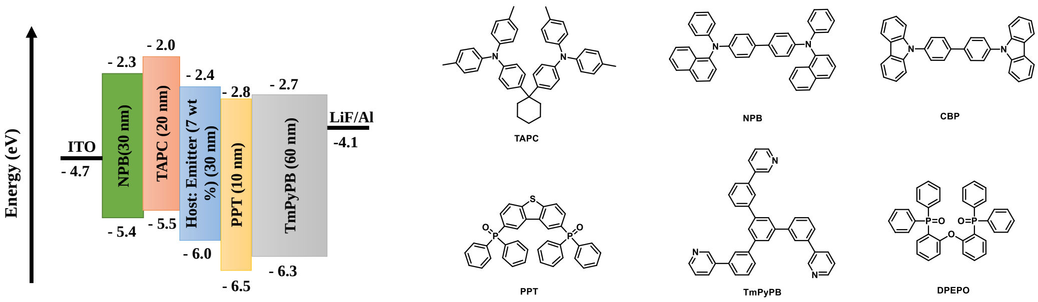


Figure S6: Schematic representation of device architecture along with molecular structures of materials

10. Comparison of PL and EL spectra

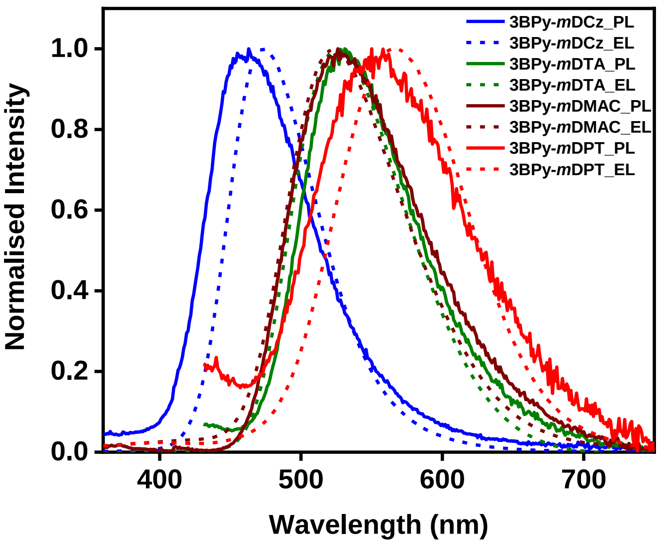
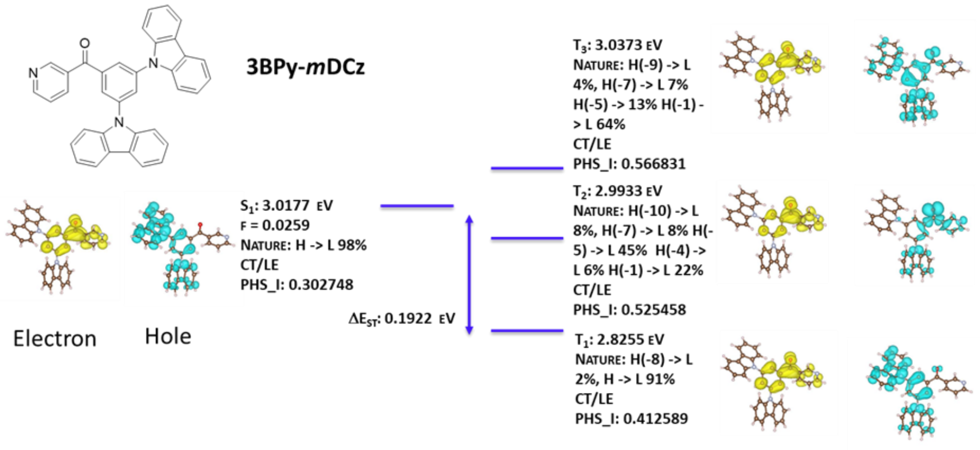
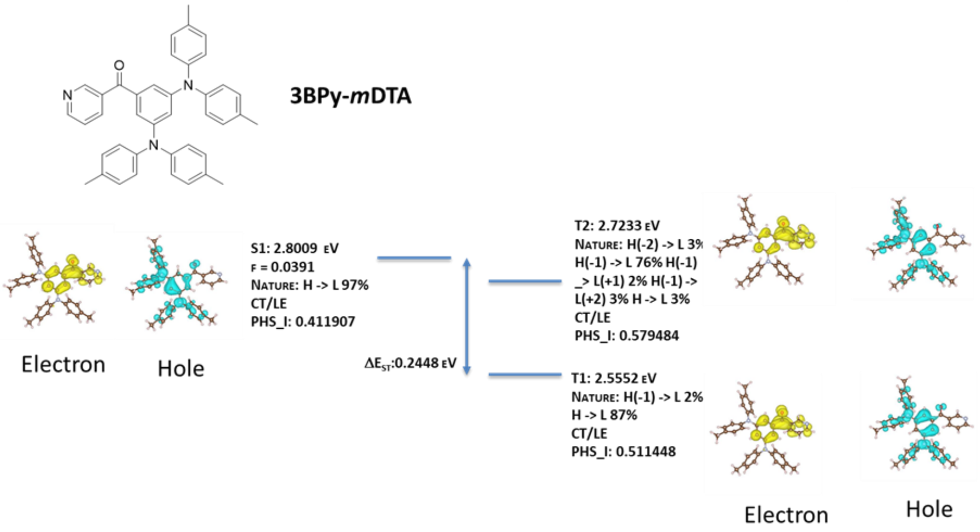


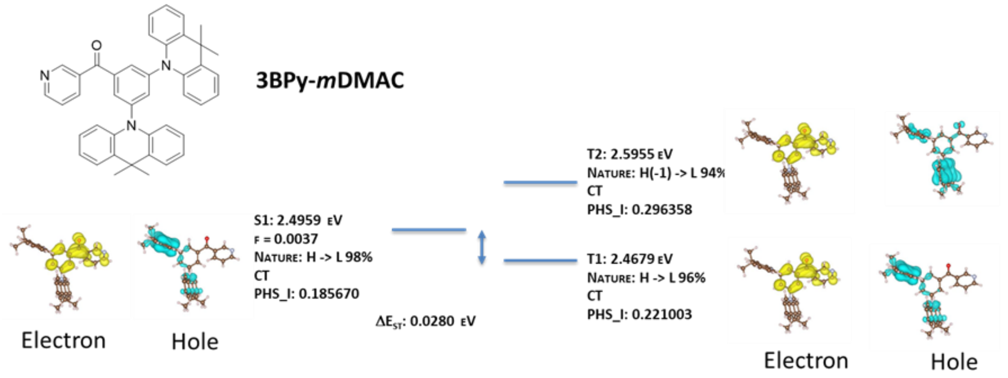
Figure S7: PL (solid) and EL (dashed) spectra in 7 wt% emitter: host doped films

11. NTO Calculations

The spatial distributions of hole-electron distributions are shown in Figure S8. The singlet and triplet excited states including hole and electron distributions were analysed using *Multiwfn* program package (Figure S8).


3BPy-*m*DCz
S₁: 3.0177 eV
F = 0.0259
Nature: H -> L 98%
CT/LE
PHS_I: 0.302748
ΔE_ST: 0.1922 eV
T₃: 3.0373 eV
Nature: H(-9) -> L 4%, H(-7) -> L 7% H(-5) -> 13% H(-1) -> L 64%
CT/LE
PHS_I: 0.566831
T₂: 2.9933 eV
Nature: H(-10) -> L 8%, H(-7) -> L 8% H(-5) -> L 45% H(-4) -> L 6% H(-1) -> L 22%
CT/LE
PHS_I: 0.525458
T₁: 2.8255 eV
Nature: H(-8) -> L 2%, H -> L 91%
CT/LE
PHS_I: 0.412589
Electron
Hole


3BPy-*m*DTA
S1: 2.8009 eV
F = 0.0391
Nature: H -> L 97%
CT/LE
PHS_I: 0.411907
ΔE_ST:0.2448 eV
T2: 2.7233 eV
Nature: H(-2) -> L 3%
H(-1) -> L 76% H(-1) _> L(+1) 2% H(-1) -> L(+2) 3% H -> L 3%
CT/LE
PHS_I: 0.579484
T1: 2.5552 eV
Nature: H(-1) -> L 2%
H -> L 87%
CT/LE
PHS_I: 0.511448
Electron
Hole
Electron
Hole


3BPy-*m*DMAC
S1: 2.4959 eV
F = 0.0037
Nature: H -> L 98%
CT
PHS_I: 0.185670
ΔE_ST: 0.0280 eV
T2: 2.5955 eV
Nature: H(-1) -> L 94%
CT
PHS_I: 0.296358
T1: 2.4679 eV
Nature: H -> L 96%
CT
PHS_I: 0.221003
Electron
Hole
Electron
Hole

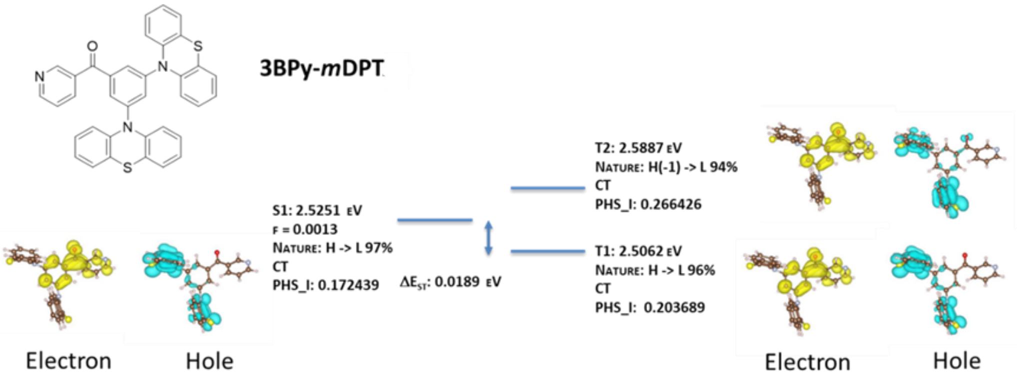

3BPy-*m*DPT
S1: 2.5251 eV
F = 0.0013
Nature: H -> L 97%
CT
PHS_I: 0.172439
ΔE_ST: 0.0189 eV
T2: 2.5887 eV
Nature: H(-1) -> L 94%
CT
PHS_I: 0.266426
T1: 2.5062 eV
Nature: H -> L 96%
CT
PHS_I: 0.203689
Electron
Hole
Electron
Hole

Figure S8: The TDDFT calculated energy diagram and the hole-electron distributions describing the excitation characters of the S_1 and T_1 excited states of 3BPy-*m*DCz, 3BPy-*m*DTA, 3BPy-*m*DMAC and 3BPy-*m*DPT respectively. The weights of the hole-electron overlap to the excitations are included. (Iso value = 0.001)

12. Calculation Formulas for the photophysical parameters

Ignoring non-radiative decay from T_1 to S_0, the rate constants in doped films can be determined using following equations: [7–9]

$$k_{P(r)} = {}^{\Phi_P}/_{\tau_P} \tag{S1}$$

$$k_{D(total)} = {}^{1}/_{\tau_D} \tag{S2}$$

$$k_{P(Total)} = k_{P(r)} + k_{IC} + k_{ISC} = {}^{k_{P(r)}}/_{\Phi_P} = {}^{1}/_{\tau_P} \tag{S3}$$

$$k_{ISC} = {}^{\Phi_D k_{P(total)}}/_{\Phi_{PL}} \tag{S4}$$

$$k_{RISC} = {}^{\Phi_D k_{P(total)} k_{D(total)}}/_{k_{ISC}\Phi_P} \tag{S5}$$

where

$k_{P(r)}$ = Radiative decay rate constant of the prompt component

$k_{D(total)}$ = Total decay rate constant of the delayed component

$k_{P(total)}$ = Total decay rate constant of the prompt component

k_{IC} = Internal conversion rate constant of the prompt component

k_{ISC} = Rate constant for intersystem crossing

k_{RISC} = Rate constant for reverse intersystem crossing

13. ^{1}H and ^{13}C NMR Spectra of targeted compounds

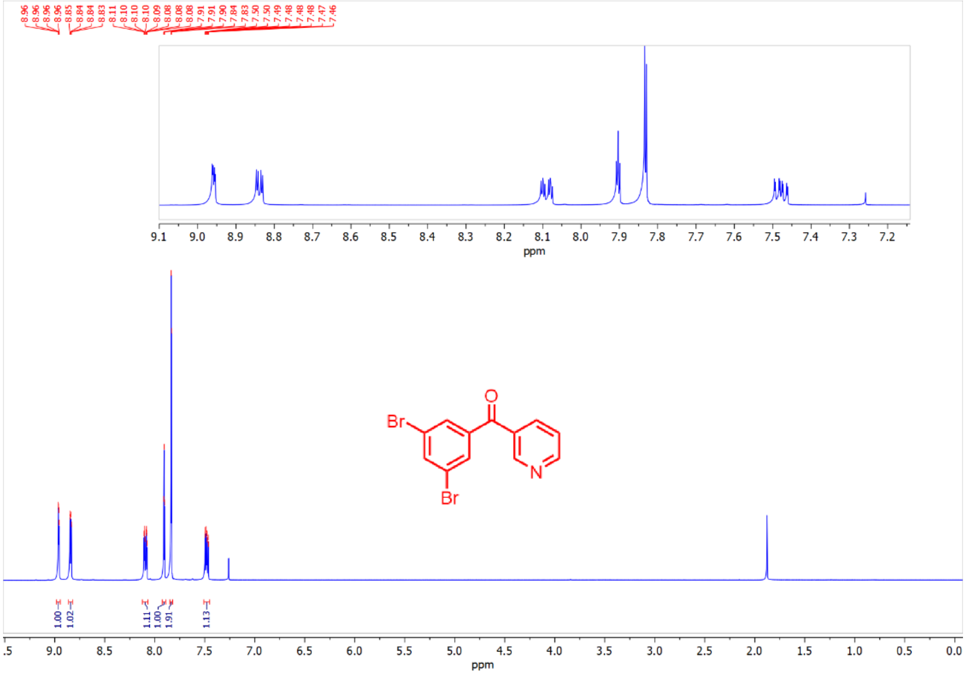


Figure S9: ^{1}H NMR of 3BPy

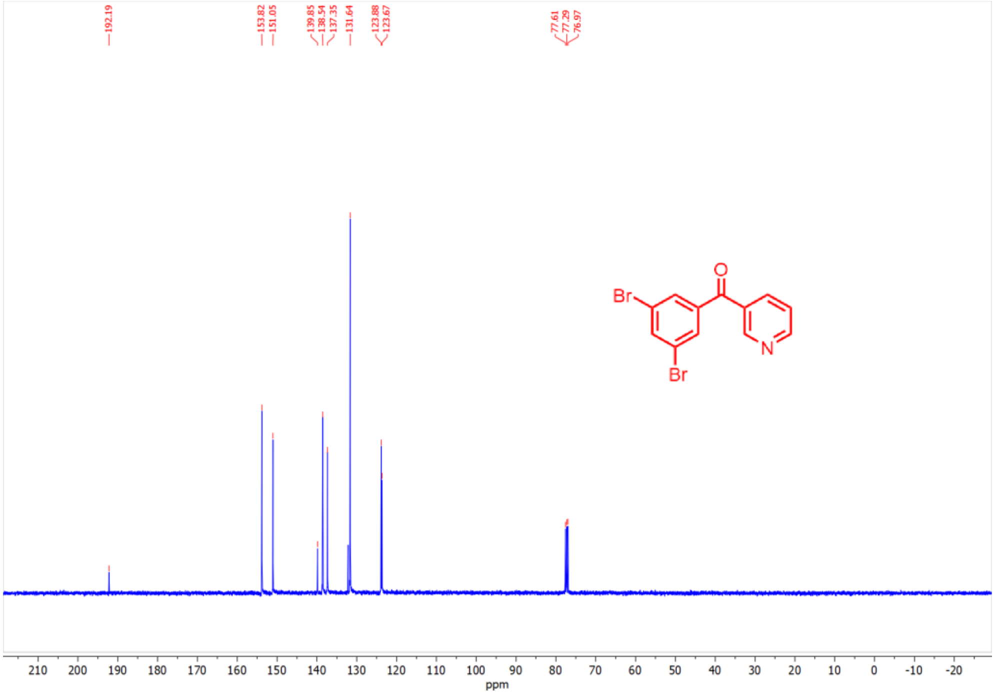


Figure S10: ^{13}C NMR of 3BPy

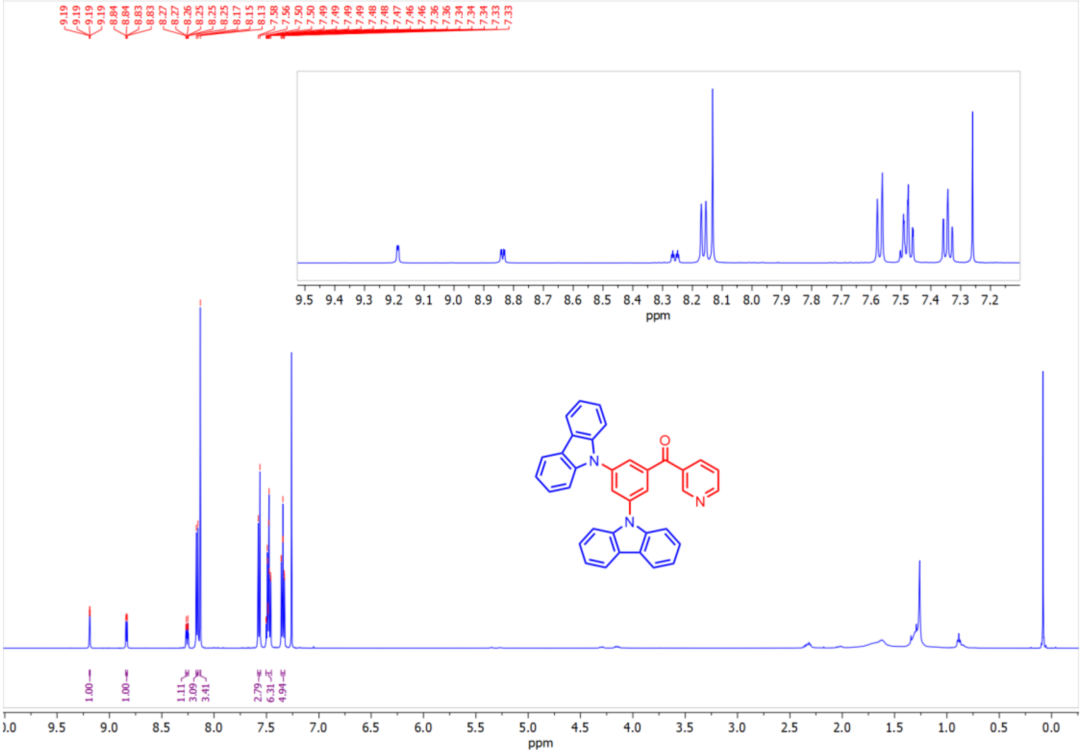


Figure S11: ^{1}H NMR of 3BPy-*m*DCz

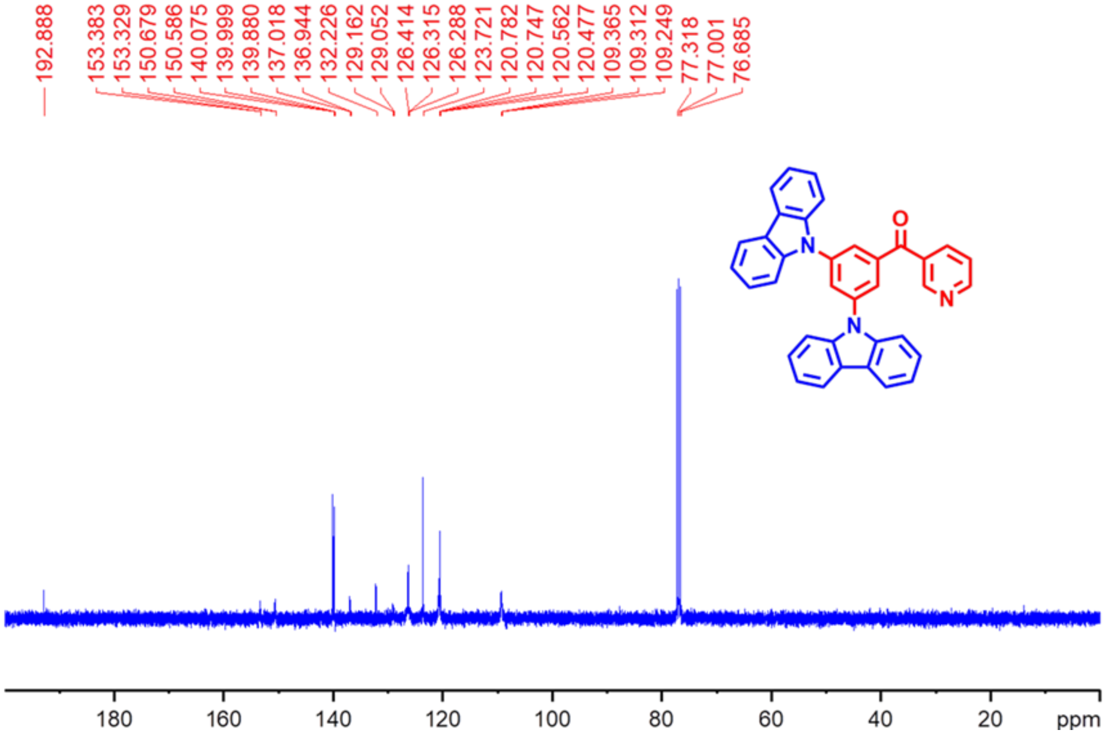


Figure S12: ^{13}C NMR of 3BPy-*m*DCz

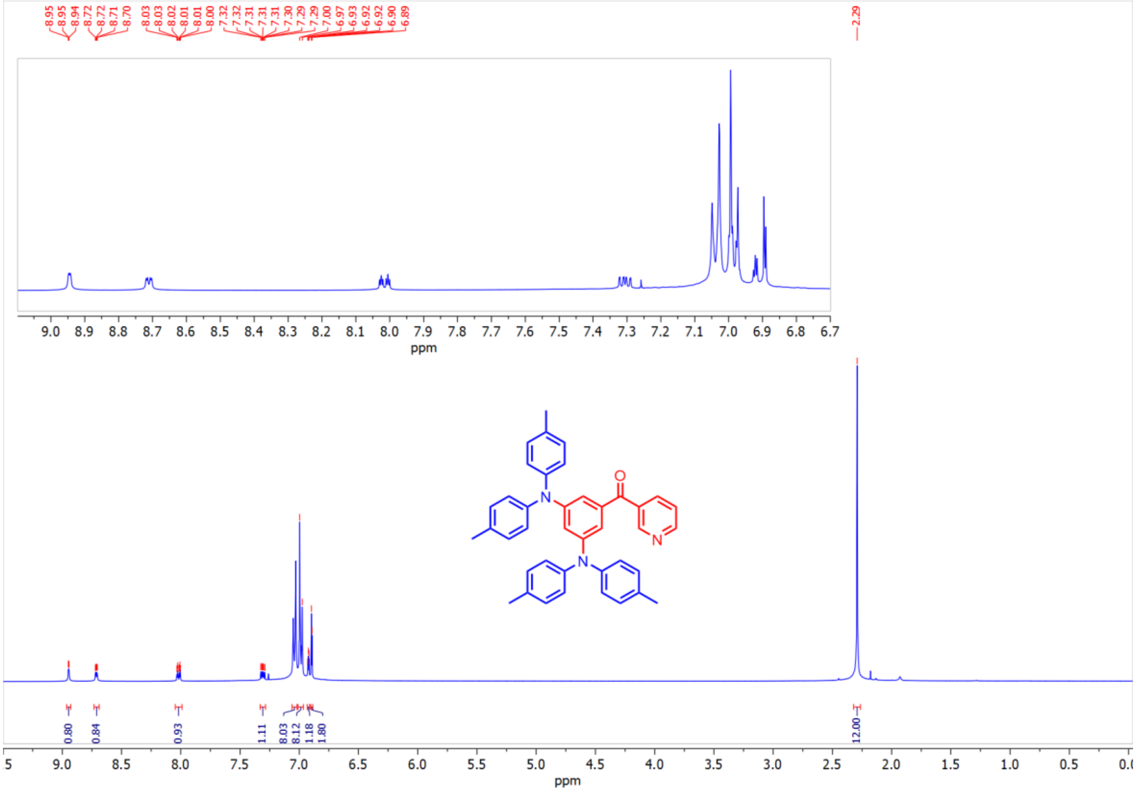


Figure S13: ^{1}H NMR of 3BPy-*m*DTA

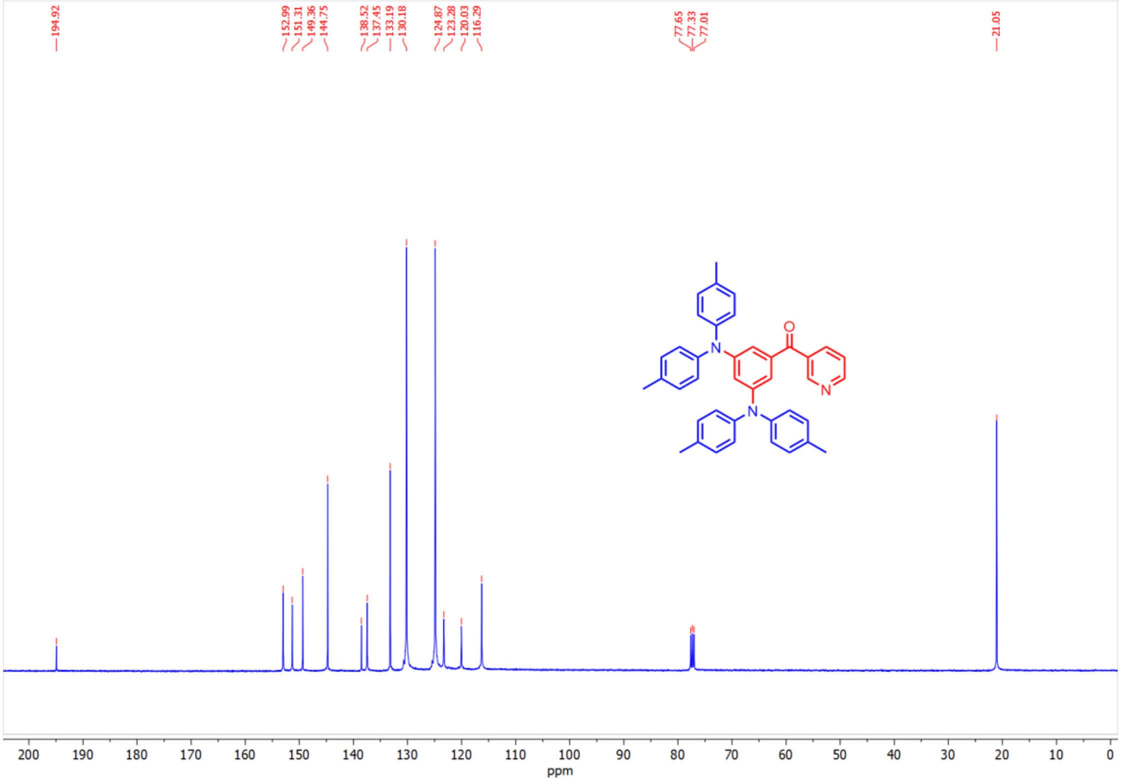


Figure S14: ^{13}C NMR of 3BPy-*m*DTA

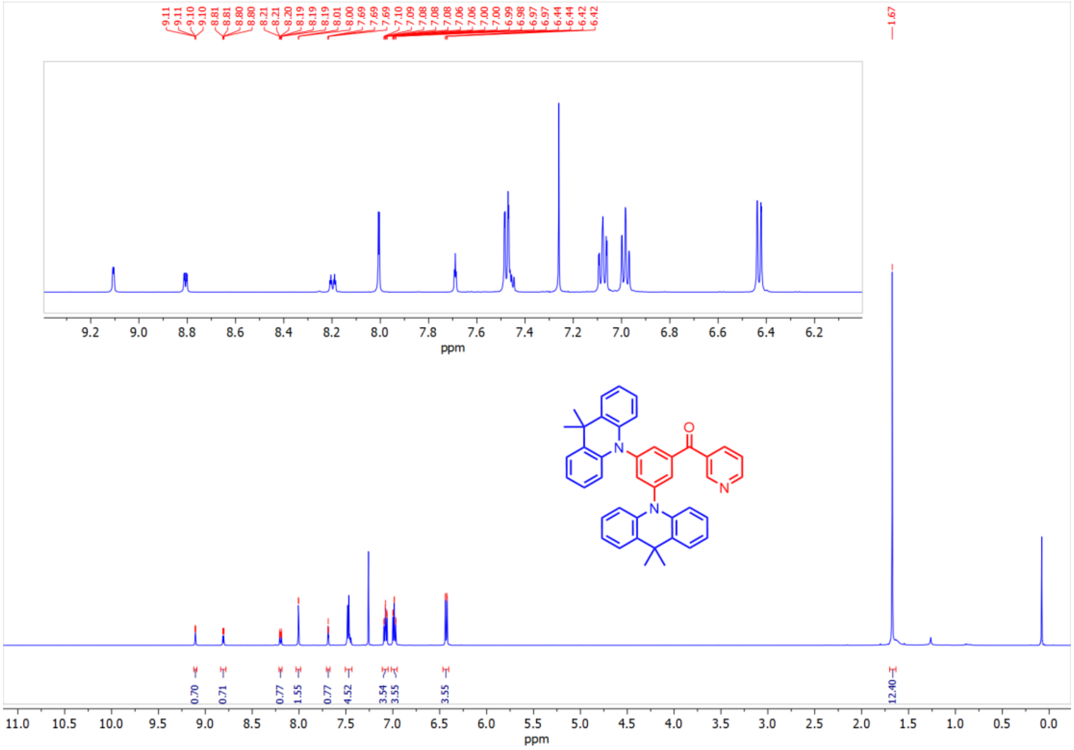


Figure S15: ^{1}H NMR of 3BPy-*m*DMAC

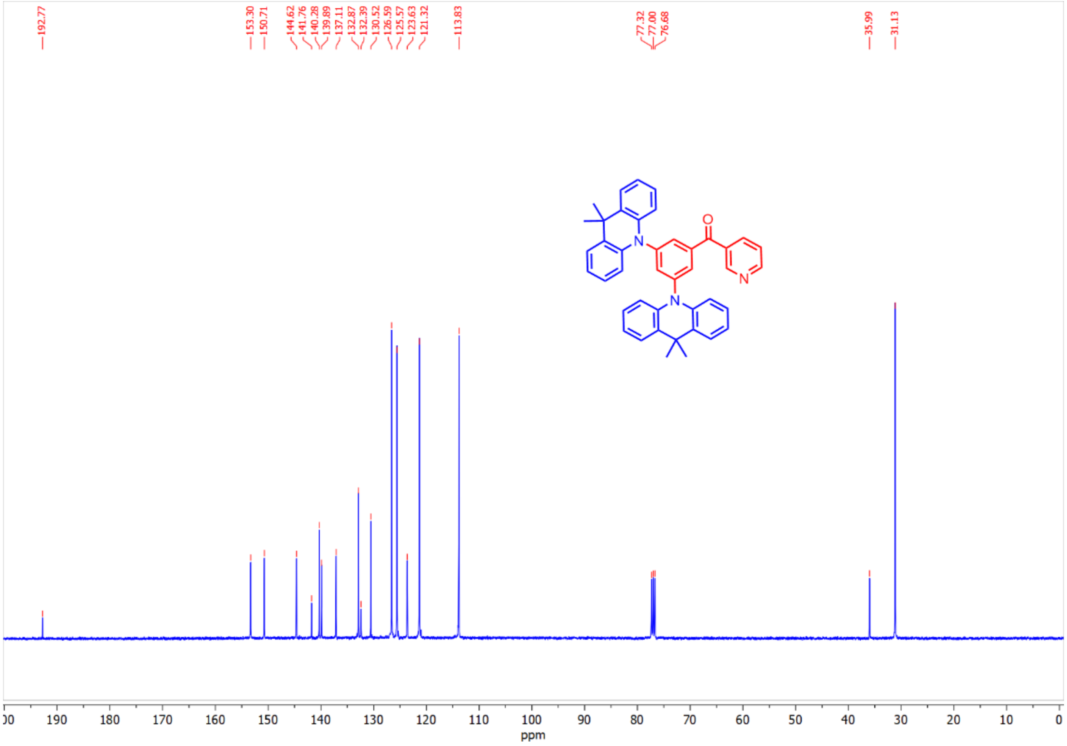


Figure S16: ^{13}C NMR of 3BPy-*m*DMAC

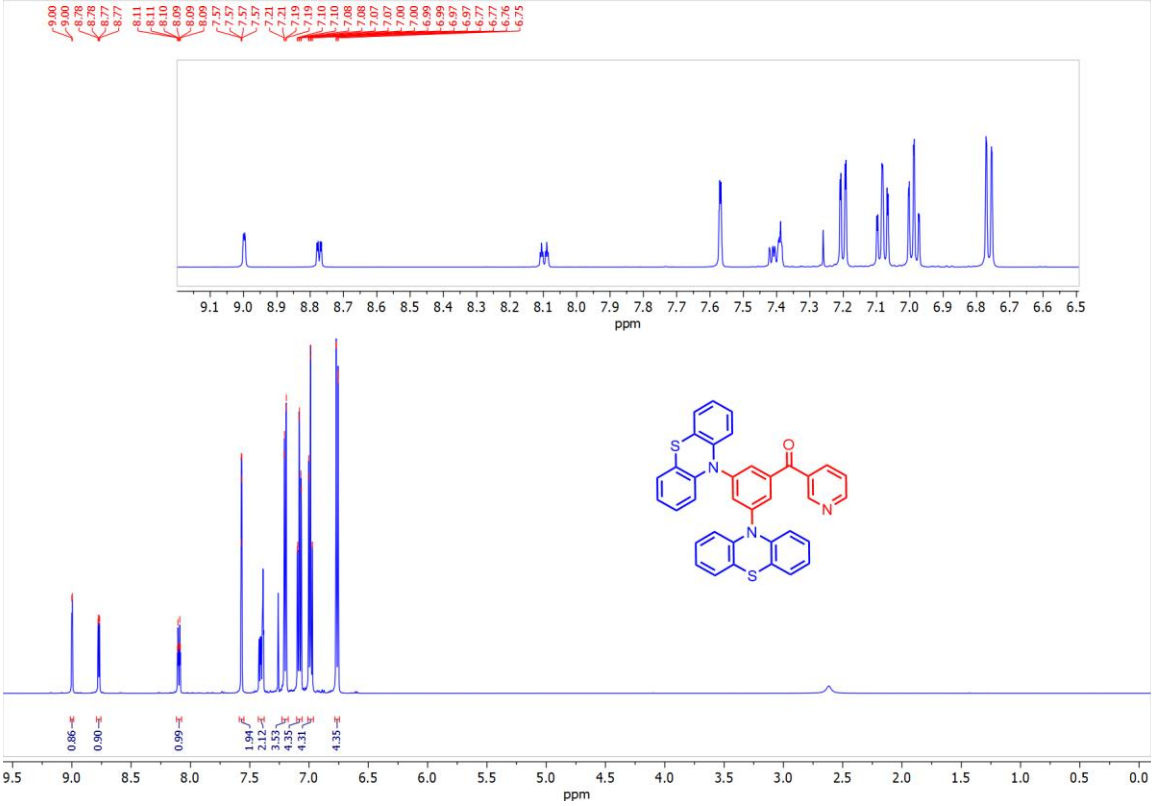


Figure S17: ^{1}H NMR of 3BPy-*m*DPT

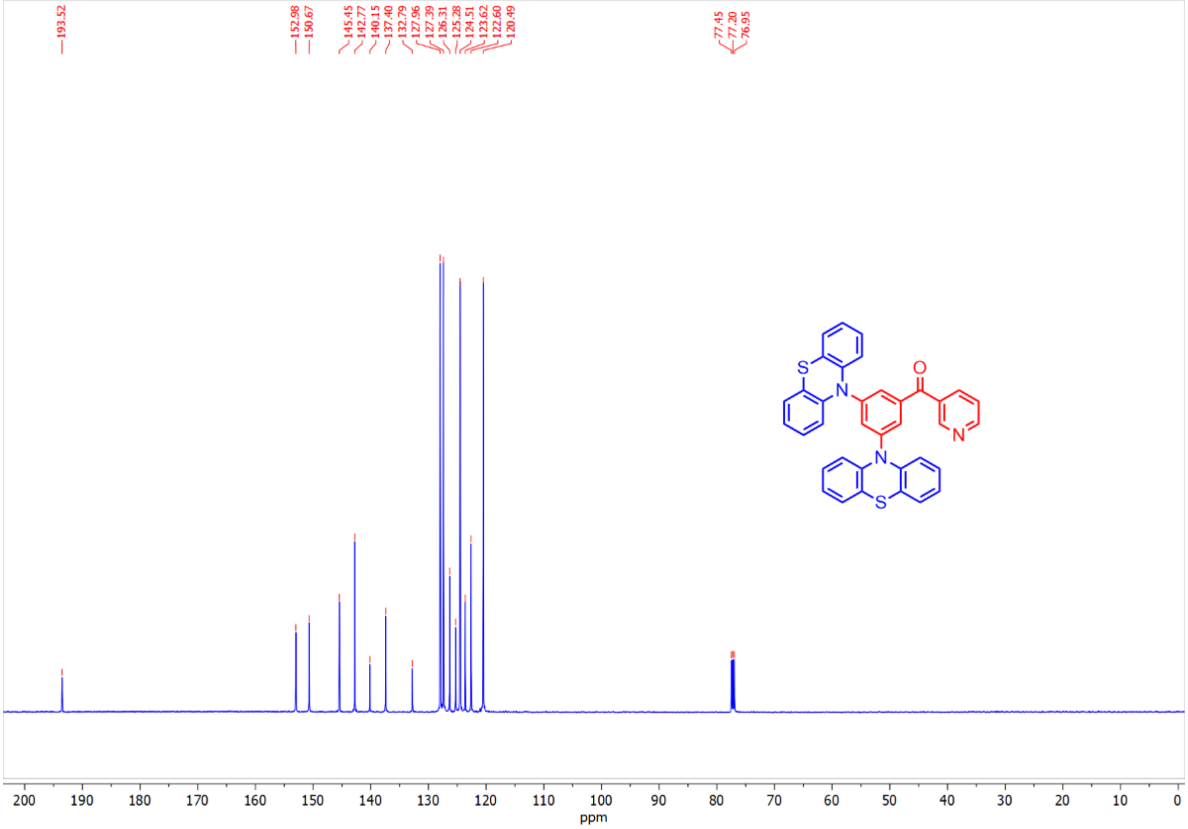


Figure S18: ^{13}C NMR of 3BPy-*m*DPT

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