Supporting information

A unique dual fluorescence emission in solid-state from small molecule based on phenanthrocarbazole with AIE luminogen as single-molecule white emissive material

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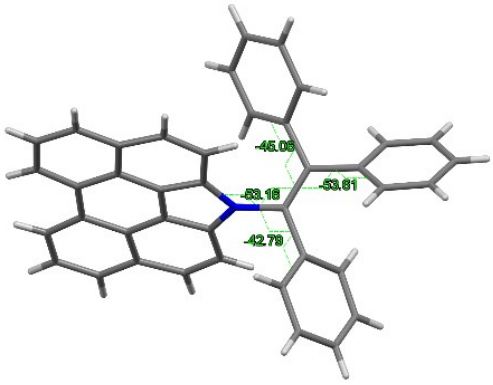
I Crystal Data and Packing

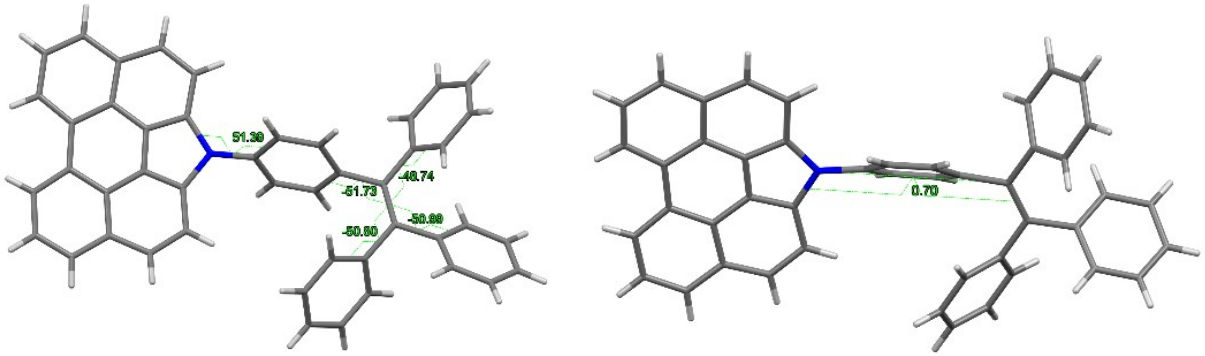
Table S1 Crystal data and structure refinement for **PCTrPE** and **PCTPE**.

Identification code	**PCTrPE**	**PCTPE**
CCDC Deposition Number	1967746	1967946
Empirical formula	$C_{40}H_{25}N$	$C_{46}H_{29}N$
Formula weight	519.61	595.70
Temperature/K	298.27	298.(2)
Crystal system	orthorhombic	orthorhombic
Space group	$P2_12_12_1$	Pbca
a/Å	9.9849(8)	9.0957(2)
b/Å	10.6568(9)	18.8991(6)
c/Å	26.012(2)	36.9438(11)
α/°	90	90
β/°	90	90
γ/°	90	90
Volume/Å^3	2767.9(4)	6350.7(3)
Z	4	8
ρ_{calc}g/cm^3	1.247	1.246

μ/mm^{-1}	0.072	0.071
F(000)	1088.0	2496.0
Crystal size/mm^3	0.45 × 0.33 × 0.25	0.450 × 0.200 × 0.120
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.37 to 57.378	5 to 50.8
Index ranges	-11 ≤ h ≤ 13, -14 ≤ k ≤ 14, -34 ≤ l ≤ 35	-10 ≤ h ≤ 10, -22 ≤ k ≤ 22, -44 ≤ l ≤ 44
Reflections collected	26512	41276
Independent reflections	7140 [R_{int} = 0.0526, R_{sigma} = 0.0595]	5811 [R_{int} = 0.0526, R_{sigma} = 0.0315]
Data/restraints/parameters	7140/0/375	5811/0/425
Goodness-of-fit on F^2	1.032	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0508, wR_2 = 0.1014	R_1 = 0.0534, wR_2 = 0.1283
Final R indexes [all data]	R_1 = 0.0851, wR_2 = 0.1125	R_1 = 0.0802, wR_2 = 0.1452
Largest diff. peak/hole / e $Å^{-3}$	0.22/-0.15	0.22/-0.23

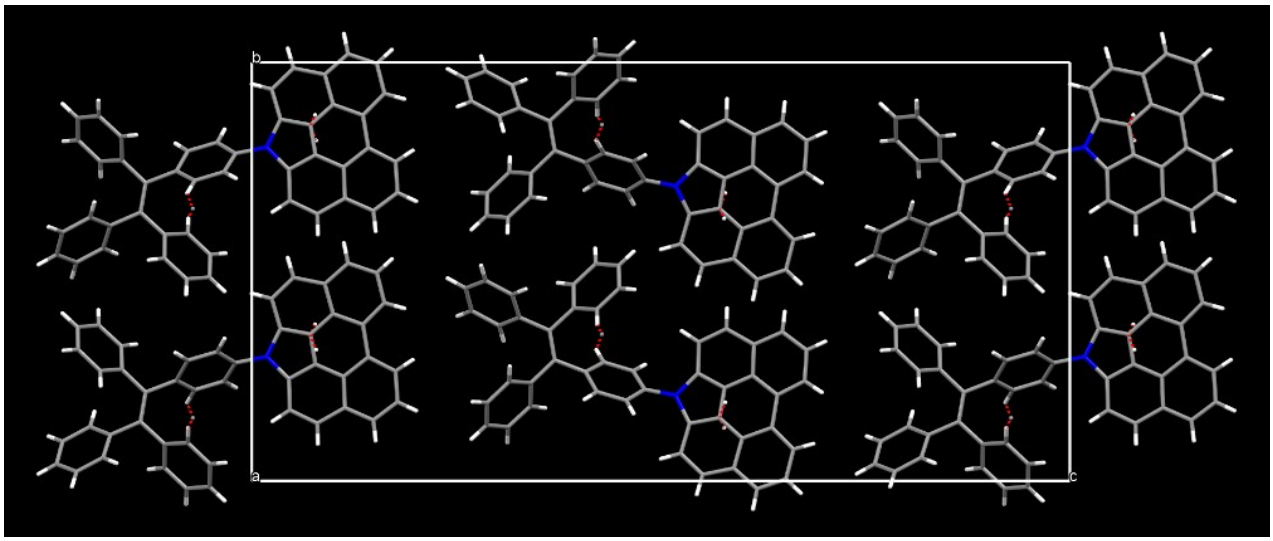


PCTrPE

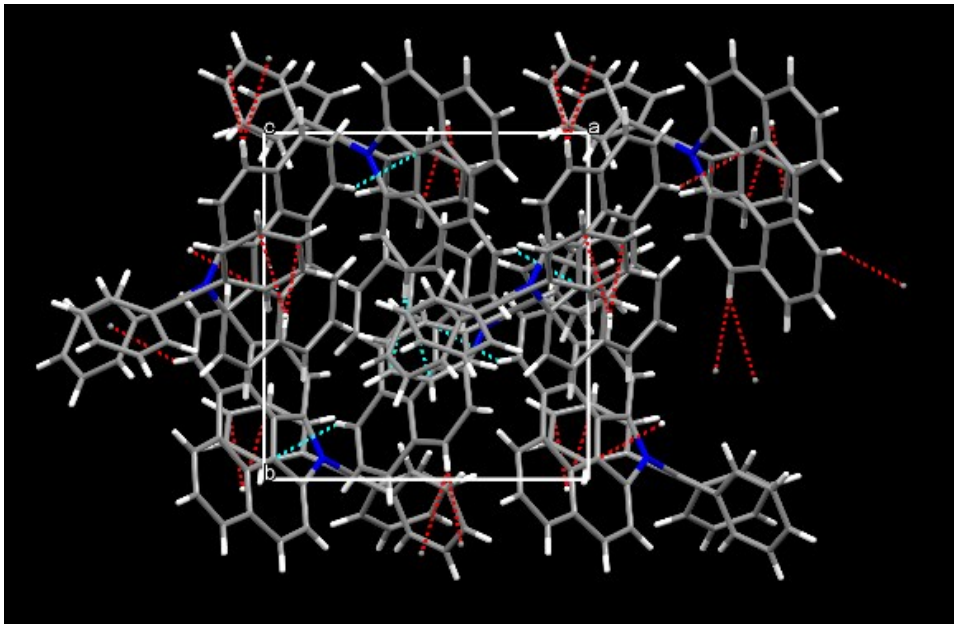


PCTPE

Figure S1. The dihedral angles (ϕ) in the molecules of **PCTrPE** and **PCTPE**.



PCTPE



PCTrPE

Figure S2. Crystal packing along *a*-axis of **PCTPE** and along *c*- axis of **PCTrPE**.

II Additional Spectra and Data

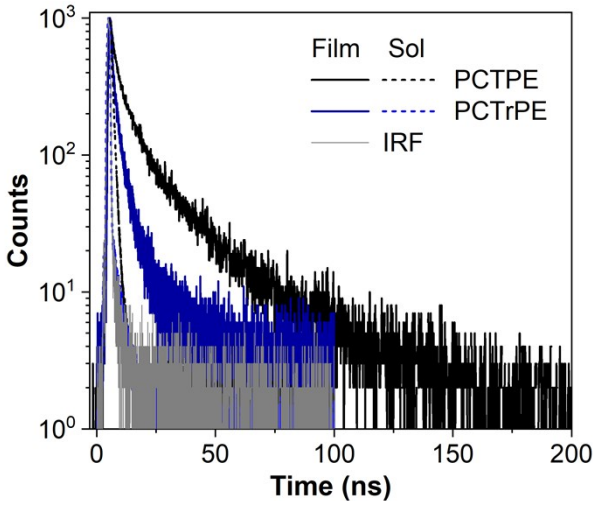


Figure S3. Transient PL spectra of **PCTPE** and **PCTrPE** in toluene solution and thin films coated on fused silica substrates.

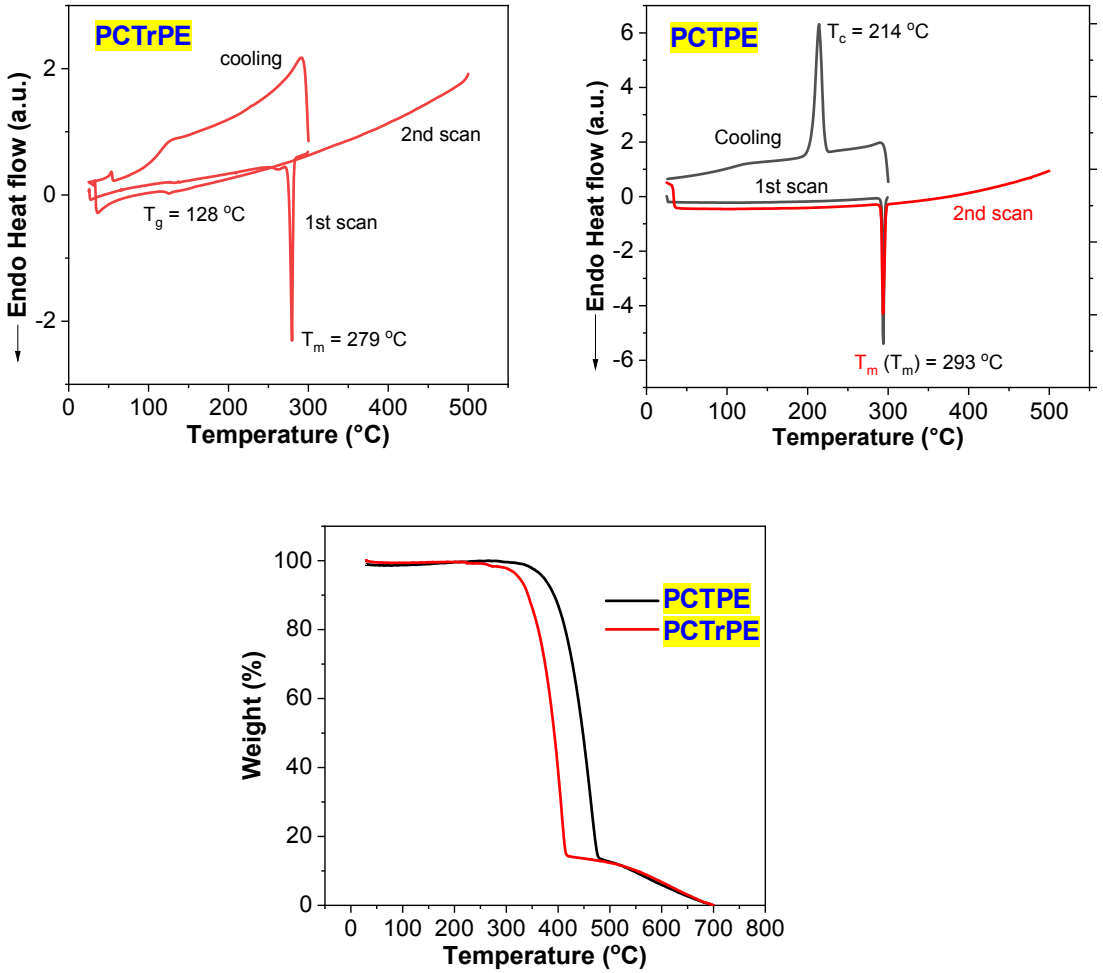


Figure S4. (Top) DSC (1st heating (thin line), cooling (dot line) and 2nd heating scans (thick line)) and (Bottom) TGA traces of **PCTPE** and **PCTrPE** analysed at heating rate of 10 °C min^{-1} under N_2 flow.

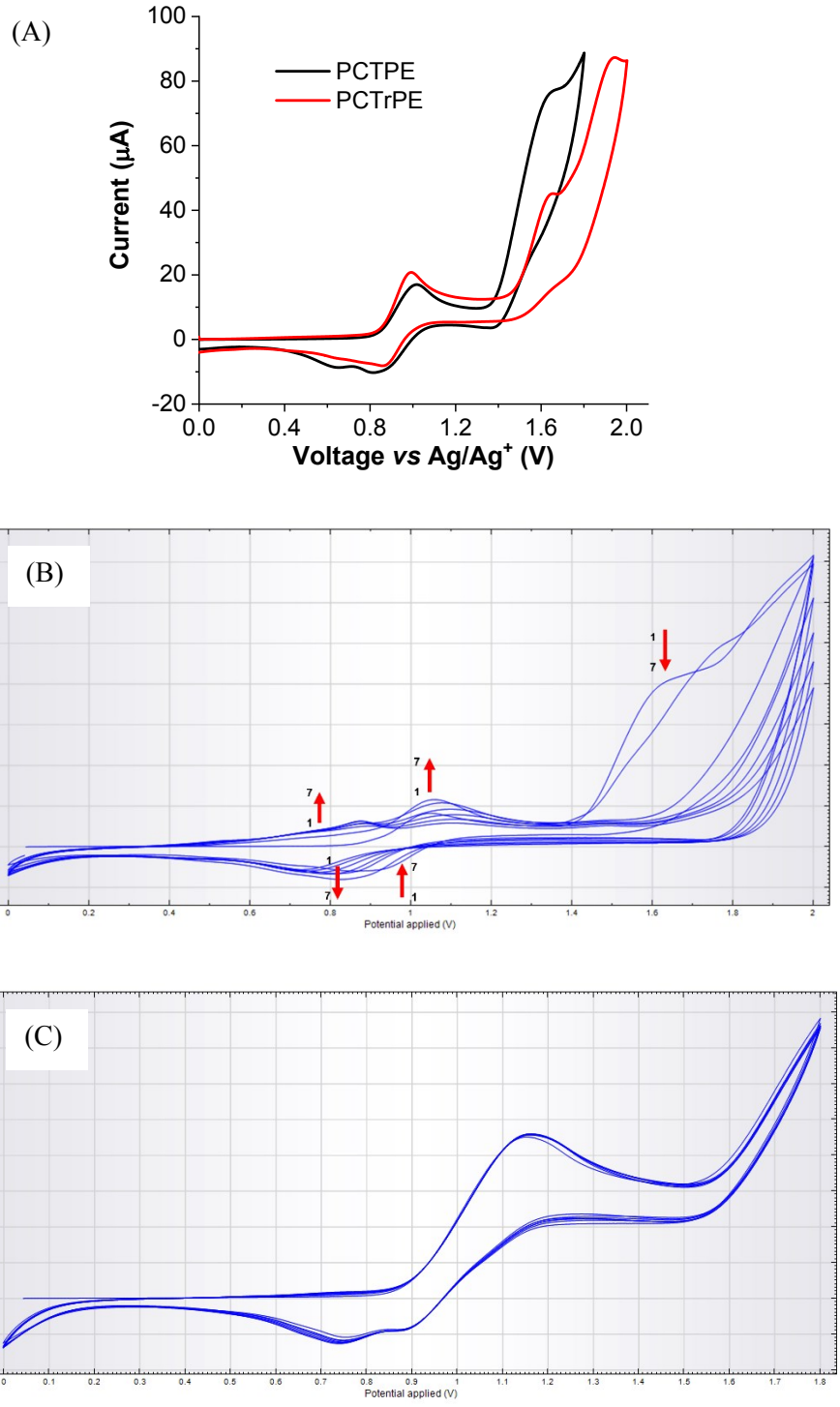


Figure S5. (A) CV plots of **PCTPE** and **PCTrPE** and (B and C) 7-scan CV plots of **PCTPE** and **PCTrPE** , respectively, measured in CH_2Cl_2 containing *n*-Bu_4NPF_6 as a supporting electrolyte at a scan rate of 50 mV s^{-1} under Ar flow. The red arrows on figure (B) showed the increasing and decreasing of working electrode's current from the 1st to 7th scans.

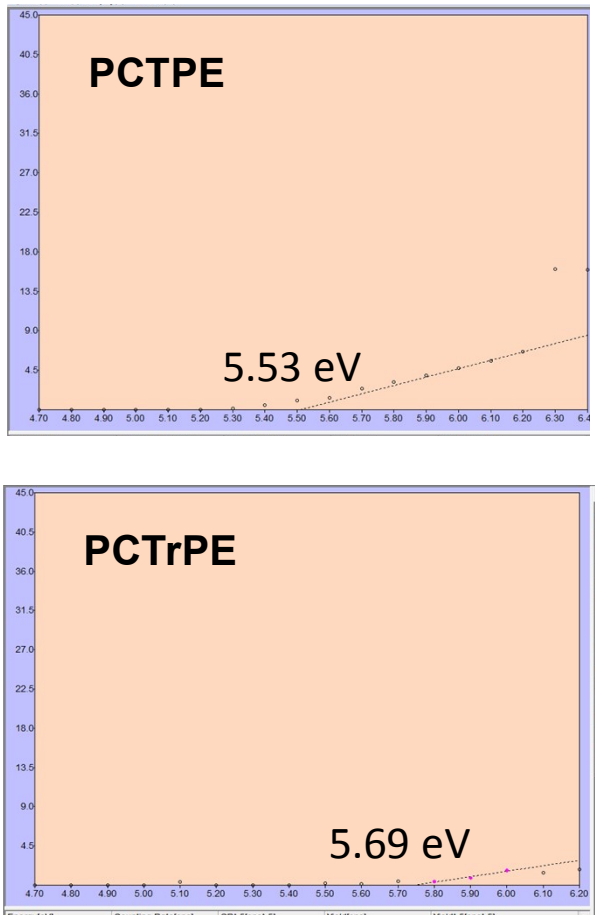


Figure S6 Photoemission yield spectroscopy in air (AC-2) spectra of **PCTPE** and **PCTrPE**.

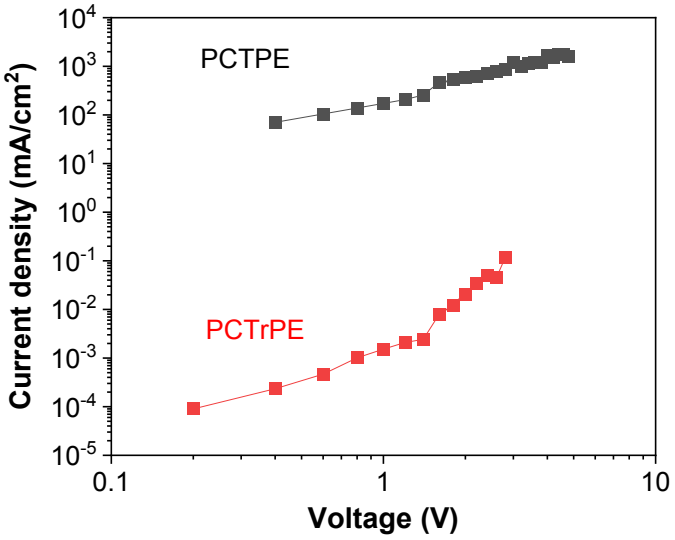


Figure S7. Current density-voltage (J-V) plot of the hole only devices: (ITO/PEDOT:PSS/**PCTPE** or **PCTrPE** (170 nm)/MoO_3/Al.

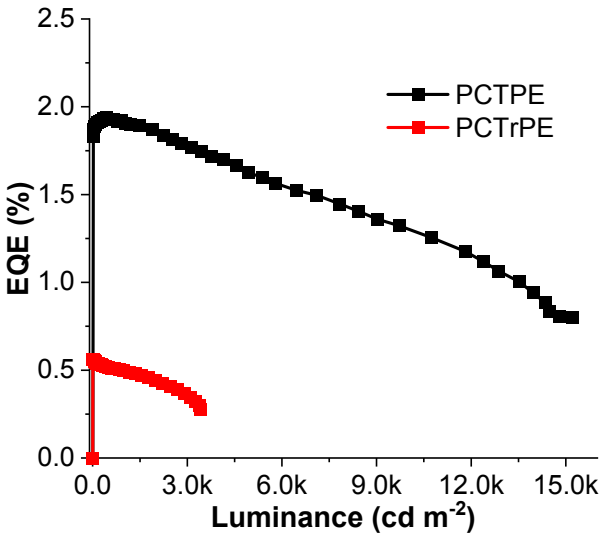
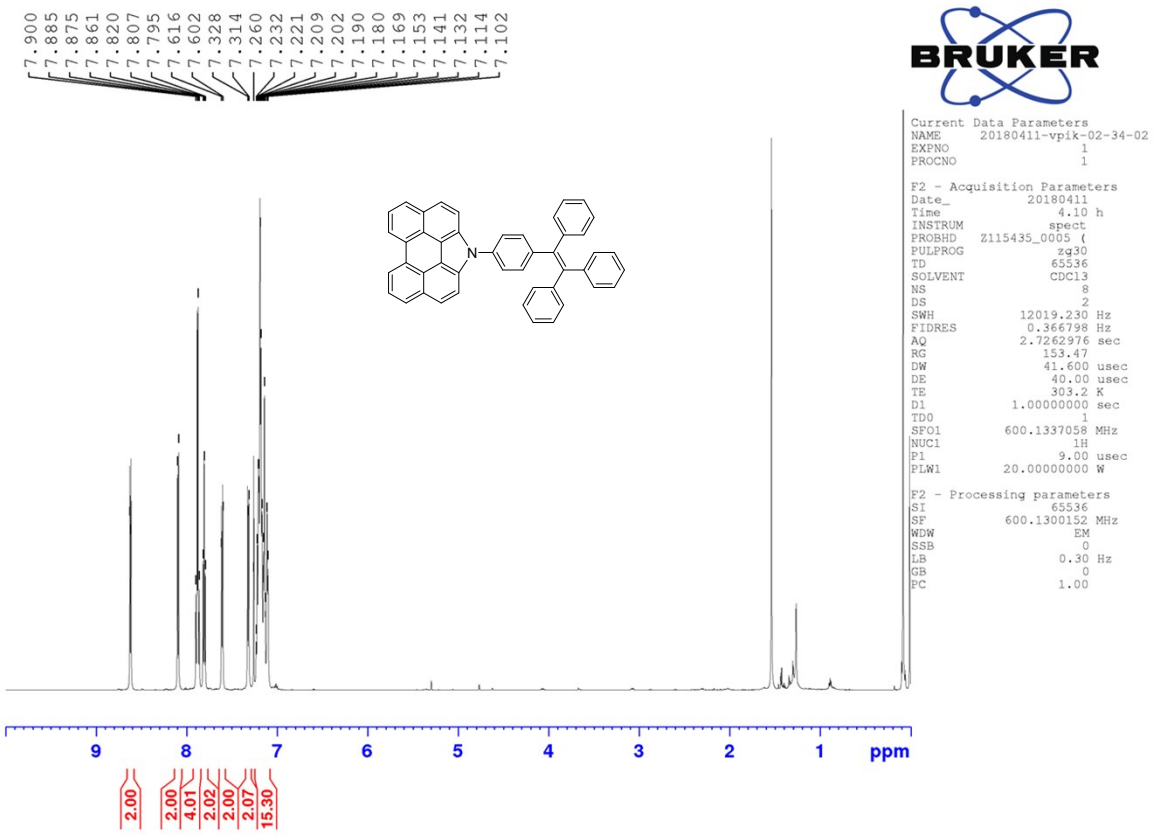


Figure S8. EQE-luminance plots of the fabricated OLEDs.

III Copies of NMR spectra and mass spectra

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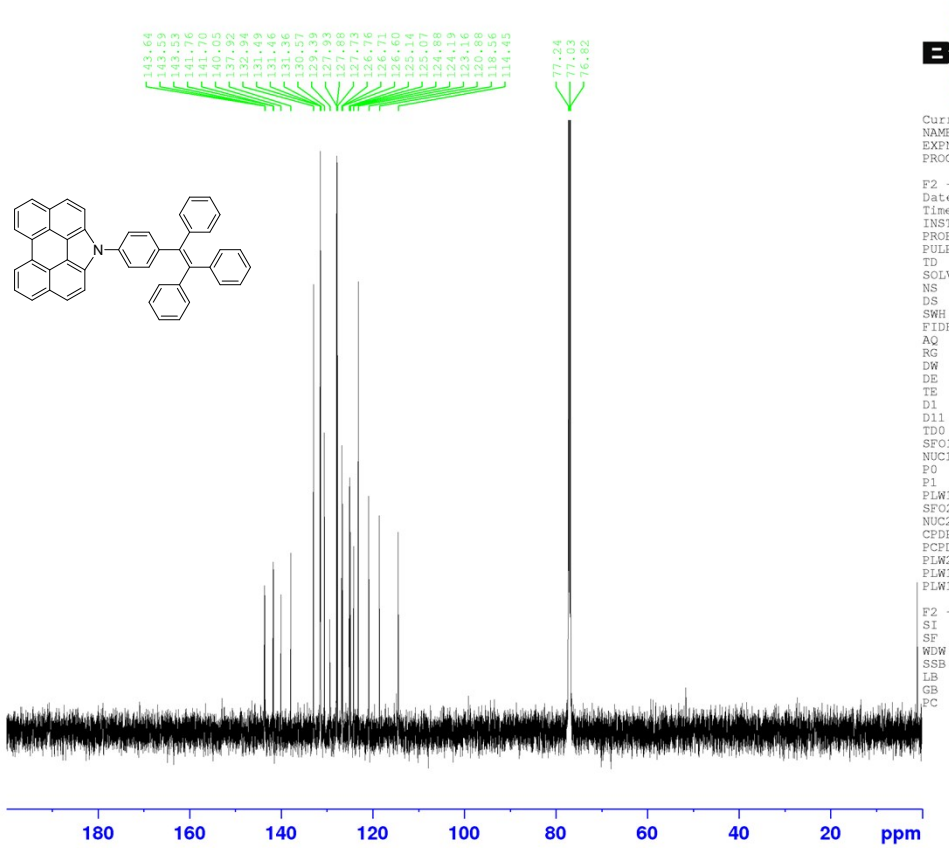


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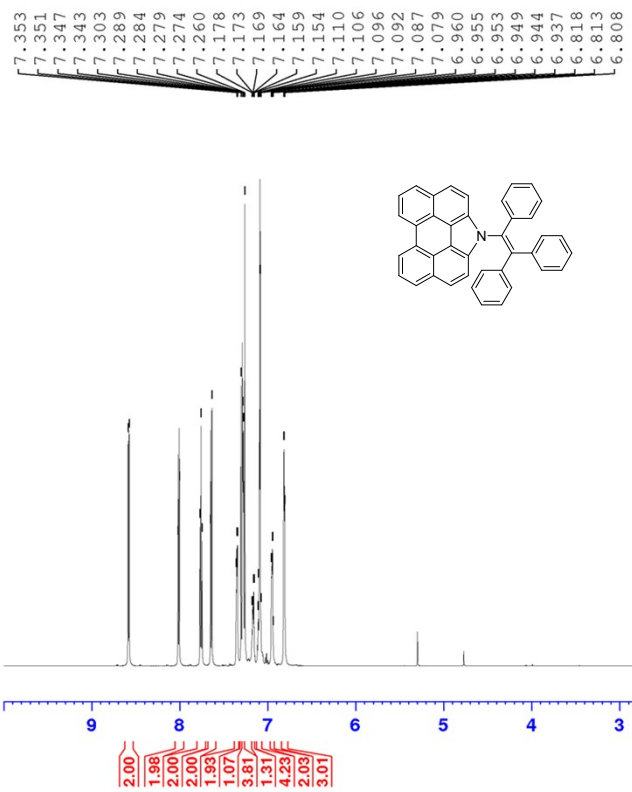

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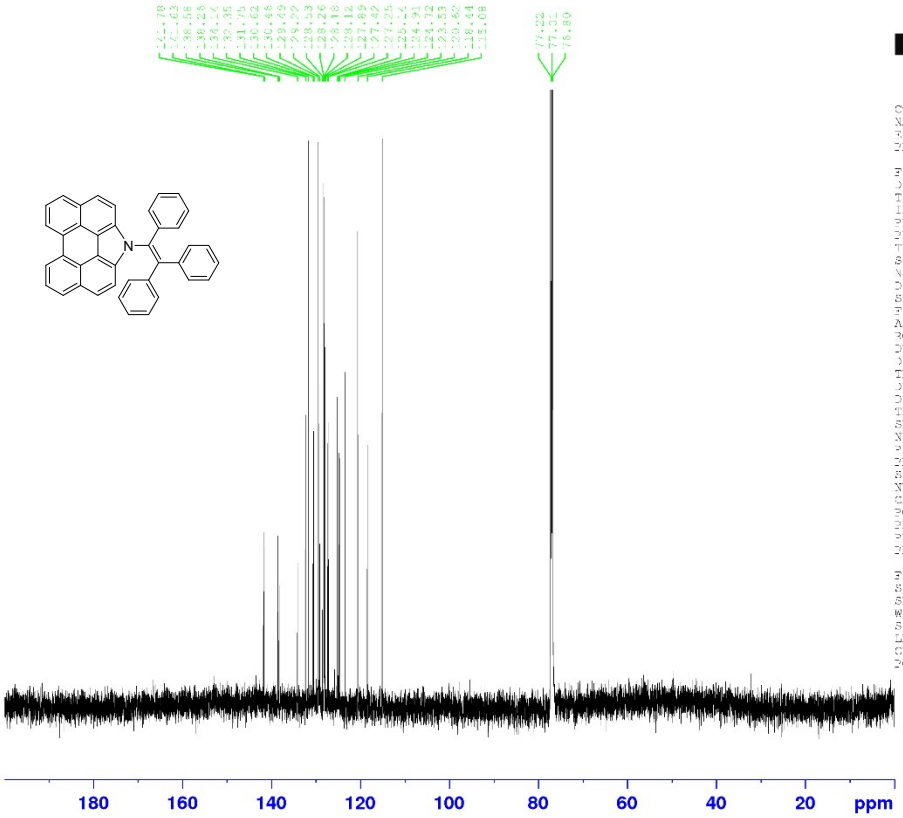

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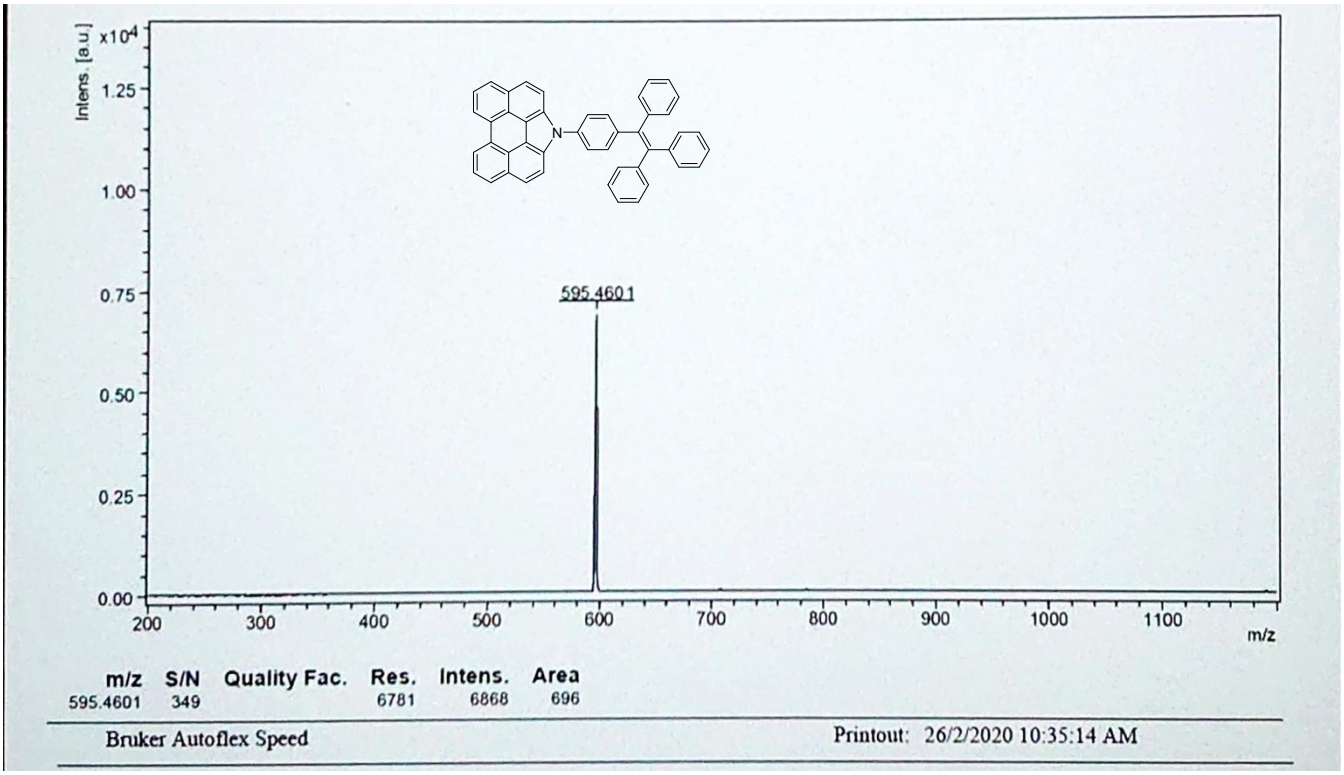
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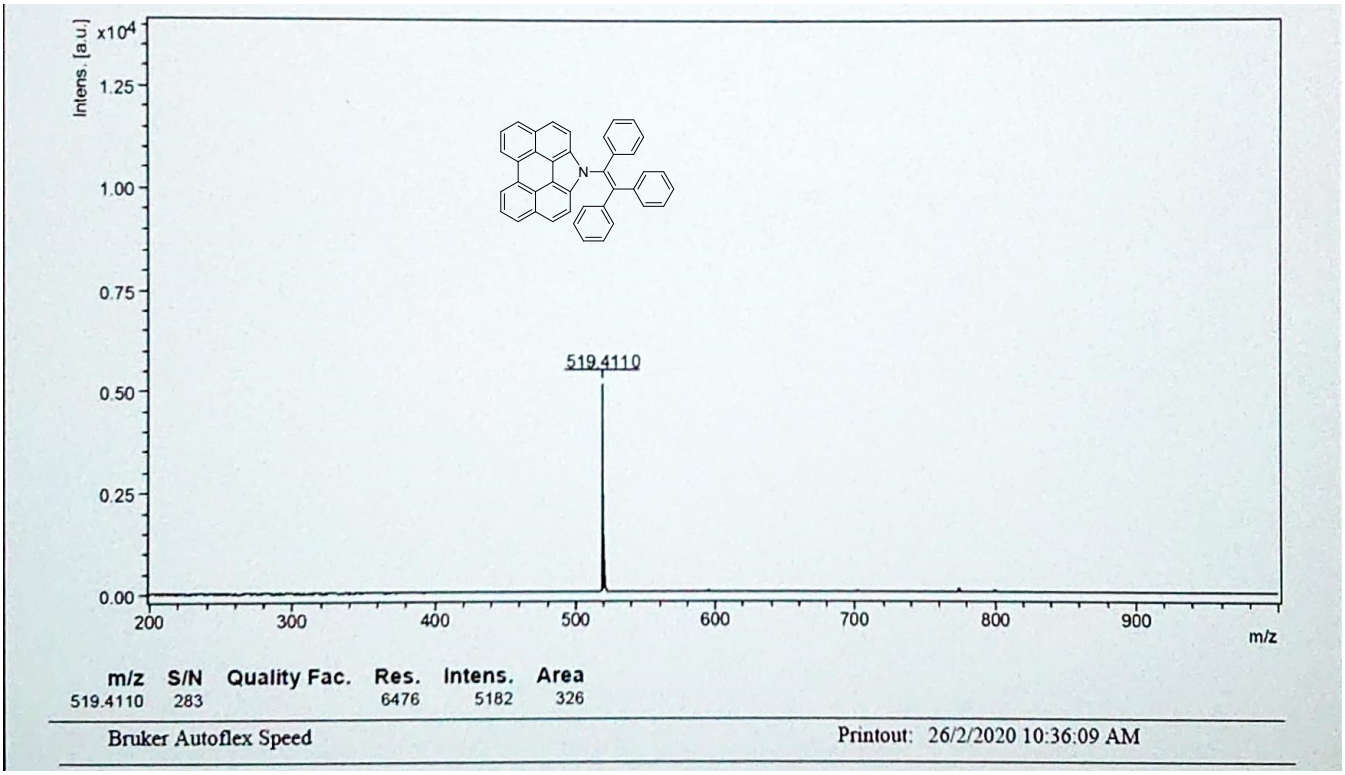
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