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Supporting Information

Efficient Pyrene-Imidazole Derivatives for Organic Light-emitting Diodes

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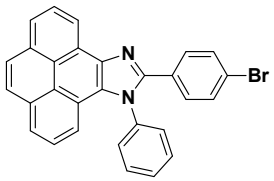
I. ^{1}H NMR, ^{13}C NMR and MS spectra of compounds.



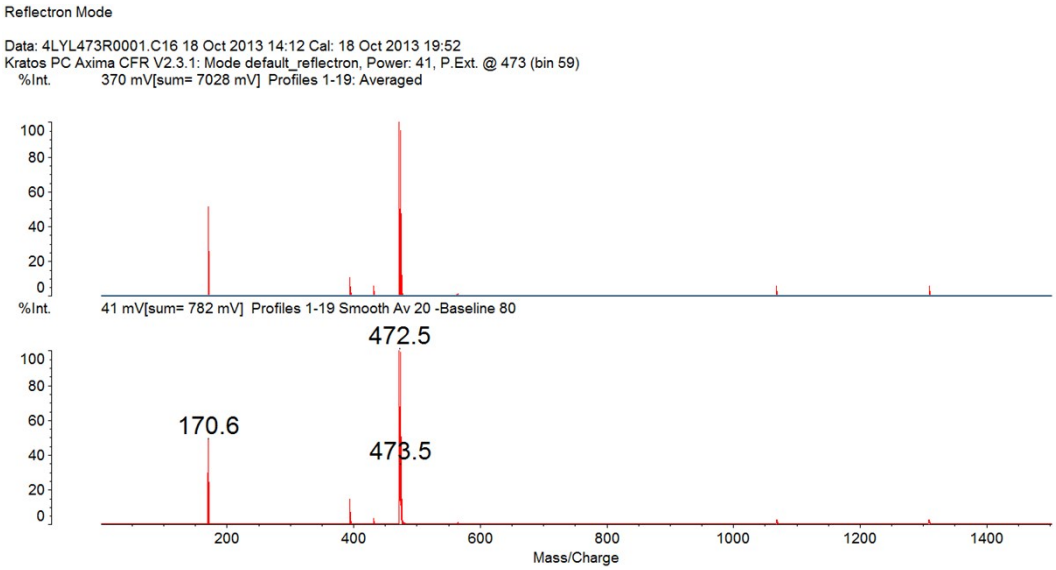
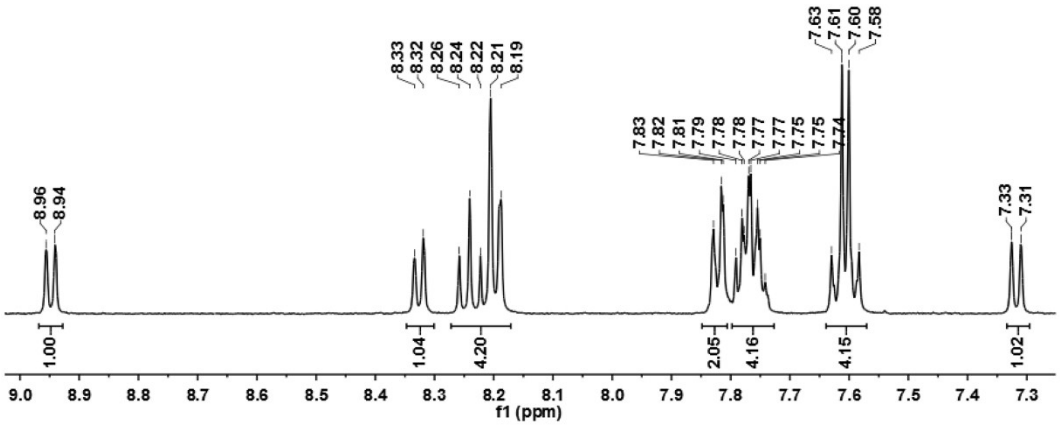
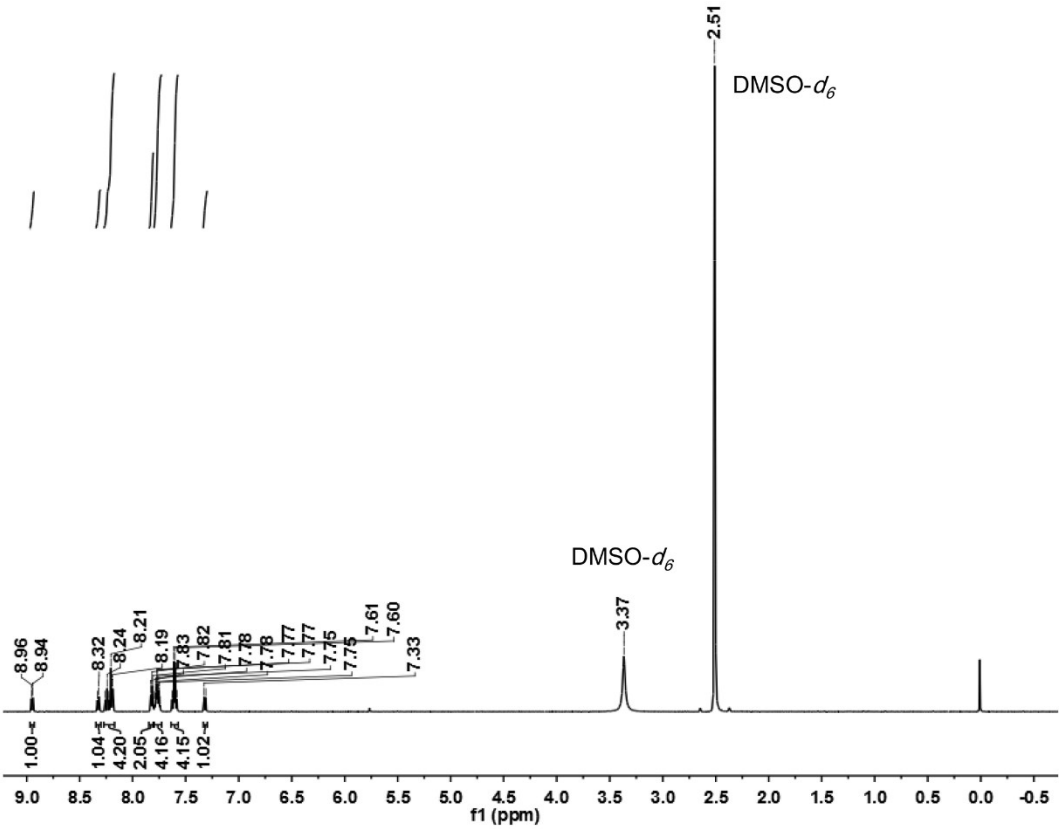


Fig. S1 Mass spectrum of compound 1.



(a)



(b)

Fig. S2 ^{1}H NMR of compound 1 measured in DMSO-d_6 with a range of -7.2 – 9.0 ppm (a) and -0.5 – 9.0 ppm (b).

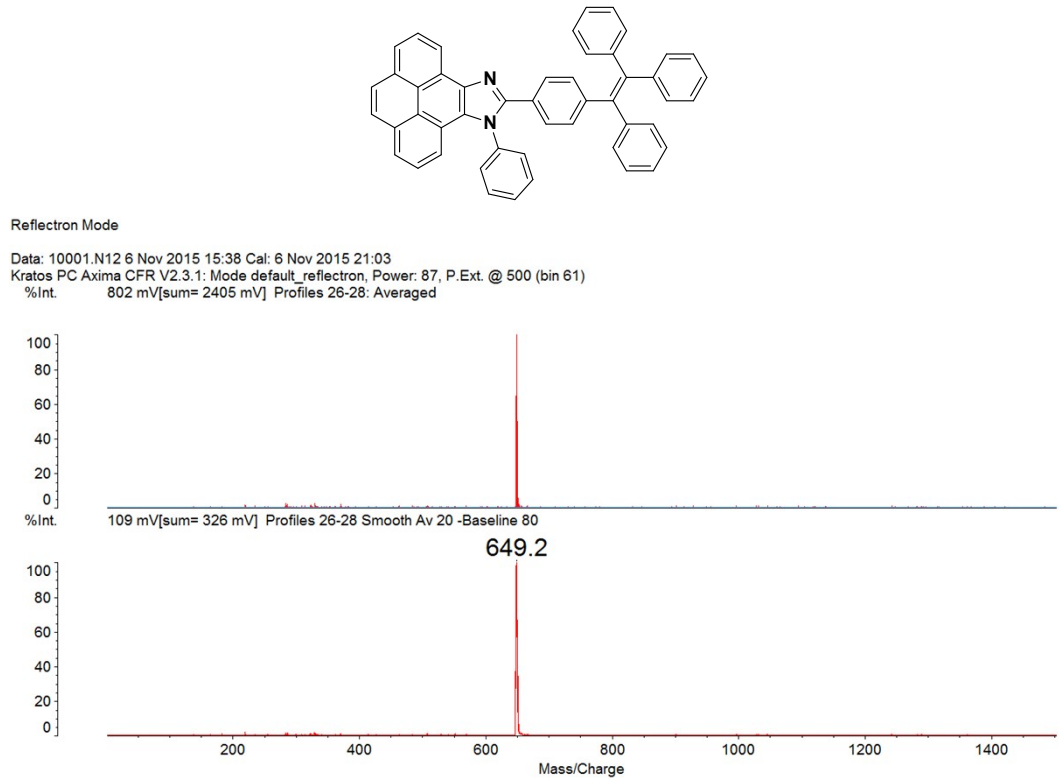
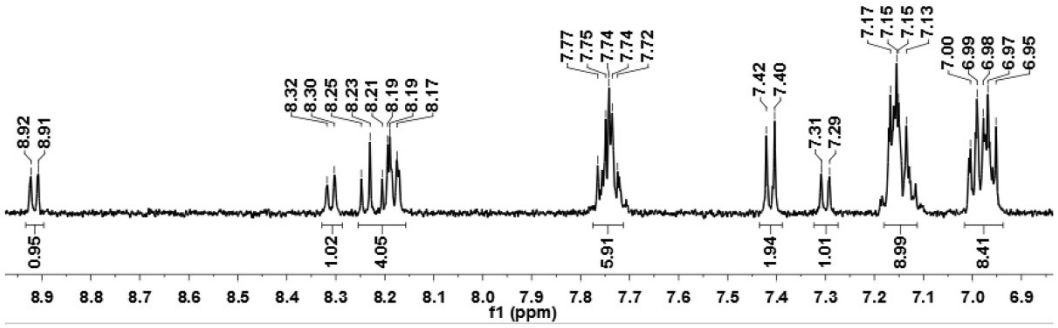
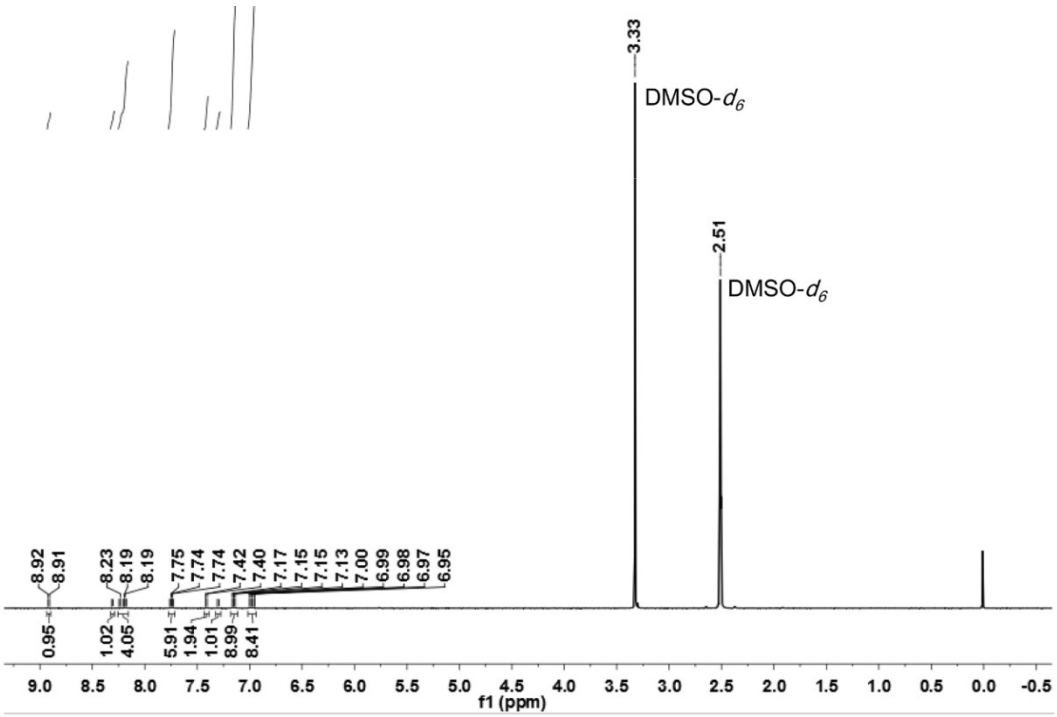


Fig. S3 Mass spectrum of compound PyTPEI.



(a)



(b)

Fig. S4 ^{1}H NMR of compound PyTPEI measured in DMSO-d_6 with a range of -6.9 – 9.0 ppm (a) and -0.5 – 9.0 ppm (b).

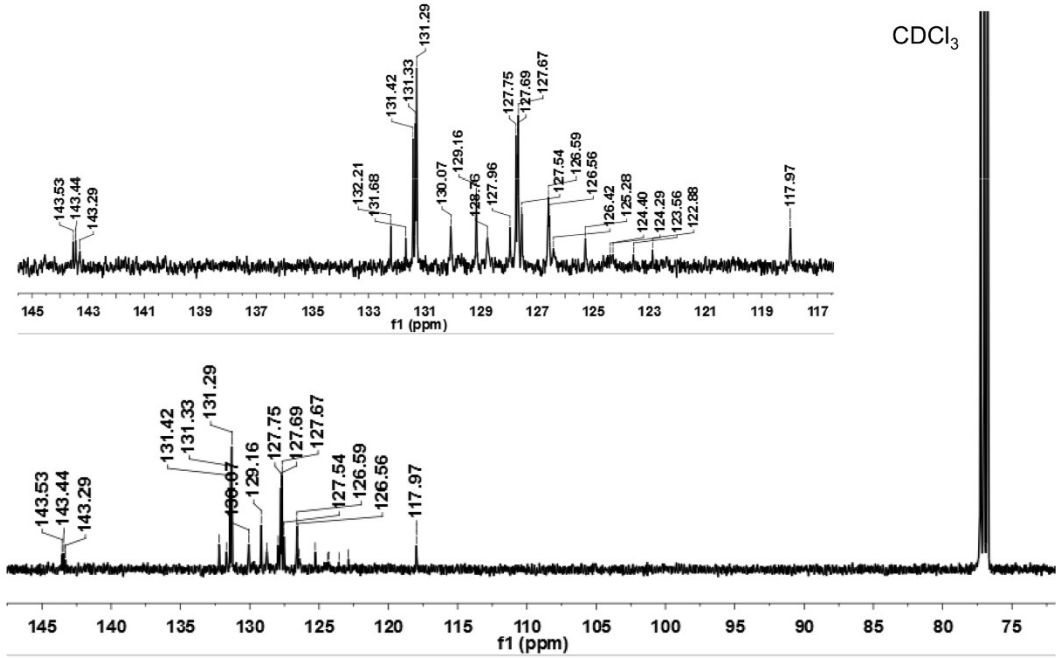


Fig. S5 ^{13}C NMR of compound PyTPEI measured in $CDCl_3$.

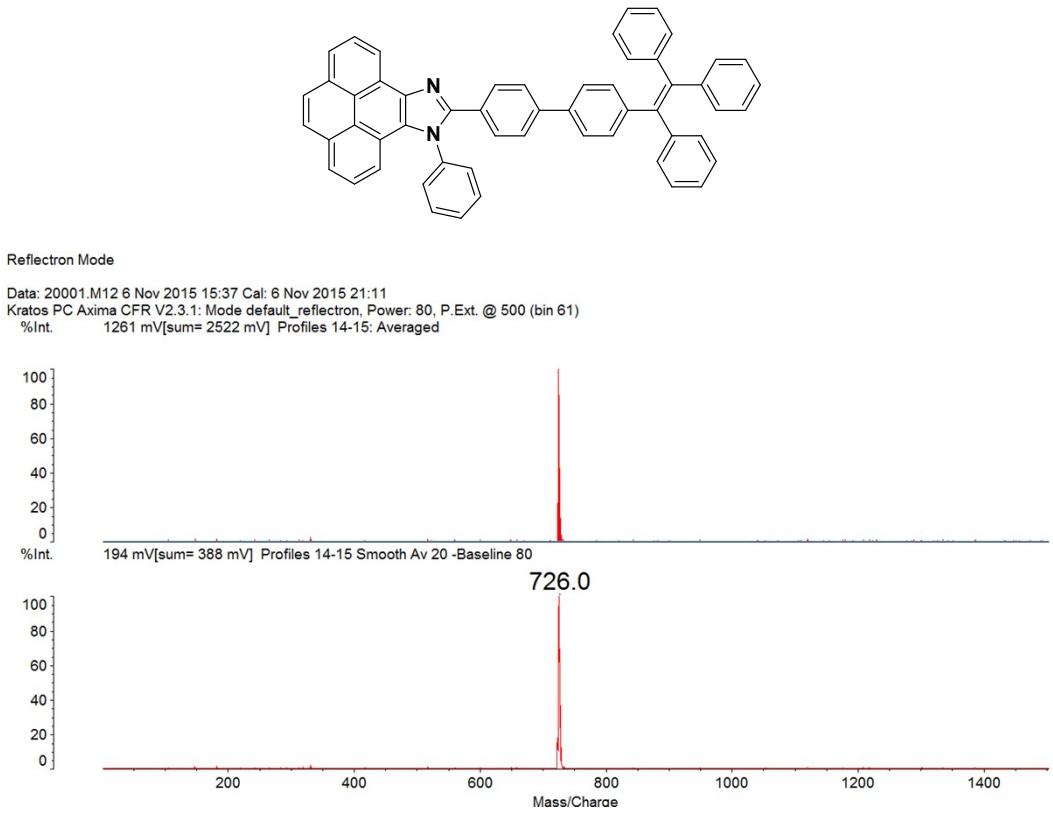
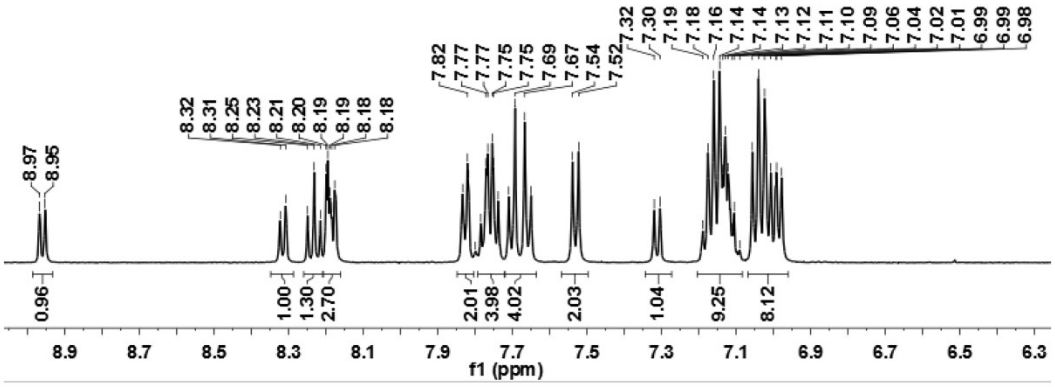
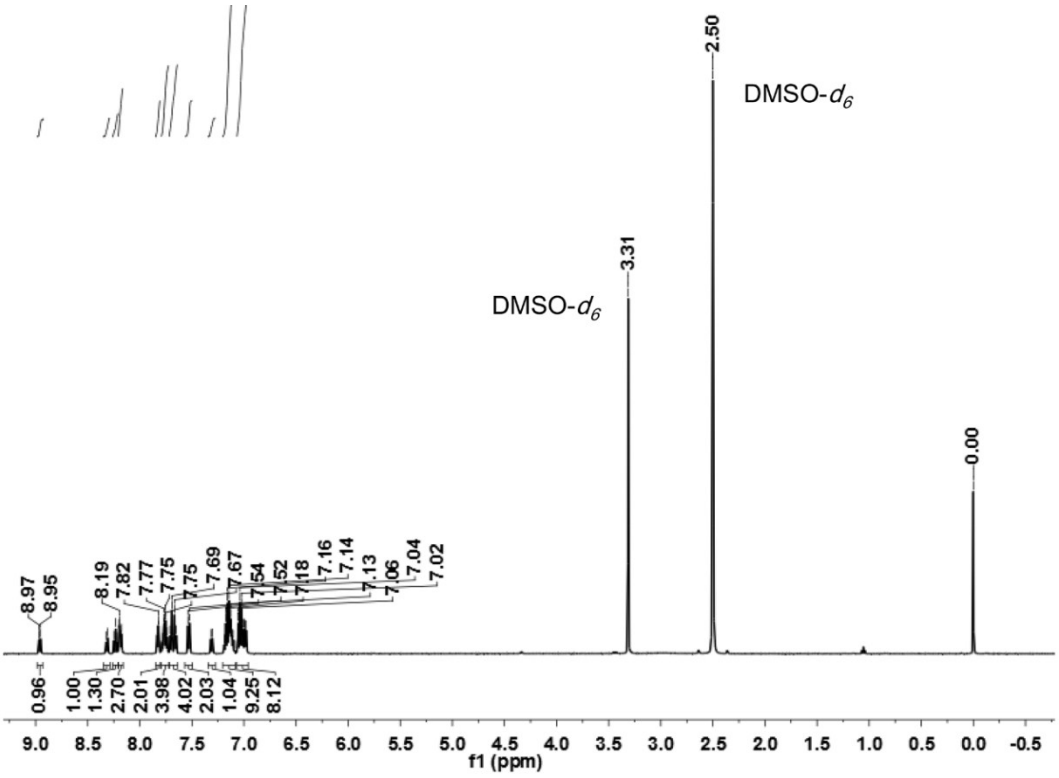


Fig. S6 Mass spectrum of compound PyPTPEI.



(a)



(b)

Fig. S7 ^{1}H NMR of compound PyPTPEI measured in DMSO-d_6 with a range of -6.9 – 9.0 ppm (a) and -0.5 – 9.0 ppm (b).

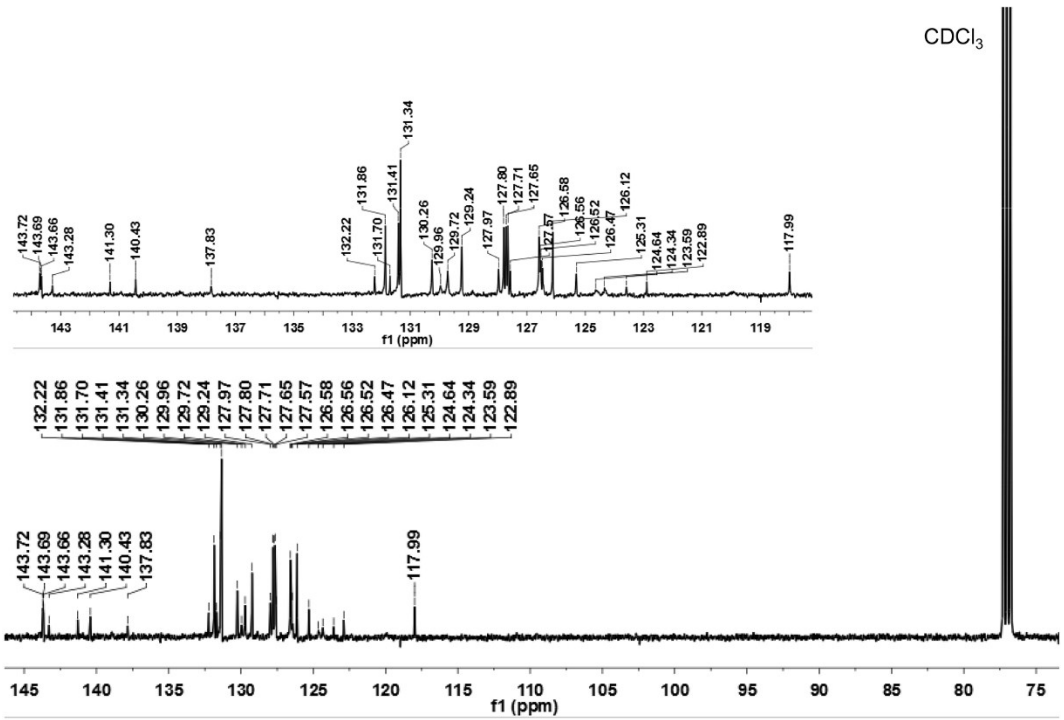


Fig. S8 ^{13}C NMR of compound PyPTPEI measured in $CDCl_3$.

II. Thermal analysis: the DSC graph of PyTPEI.

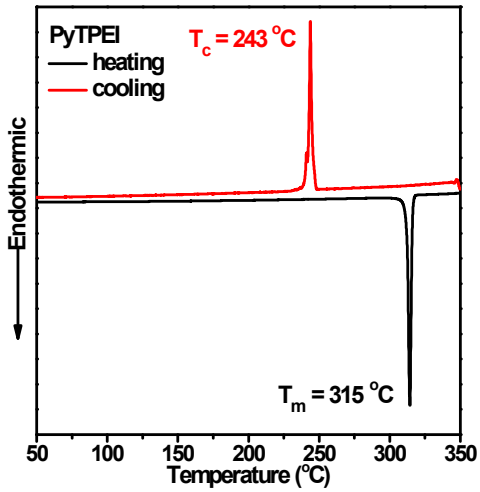


Fig. S9 DSC thermograms of PyTPEI under nitrogen at a heating rate of 10 °C min^{-1}.

III. Aggregation-induced emission properties for PyTPEI and PyPTPEI.

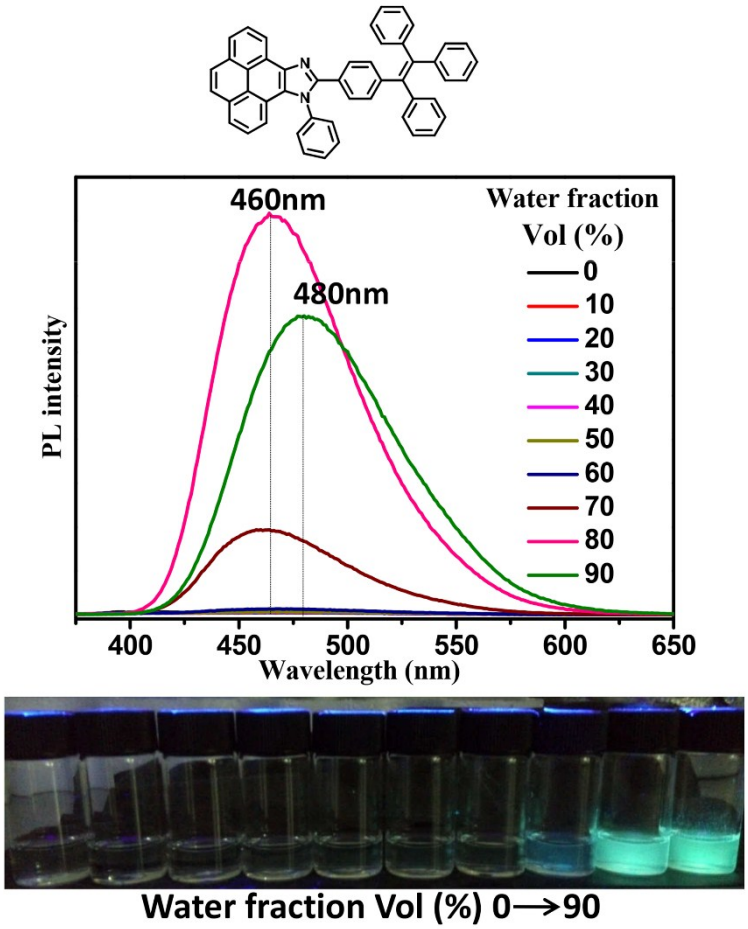


Fig. S10 Molecular structural formula of PyTPEI and PL spectra in THF/water mixtures with different water fractions (f_w) and photograph in THF–water mixtures with different water fractions (f_w) under 365 nm UV illumination.

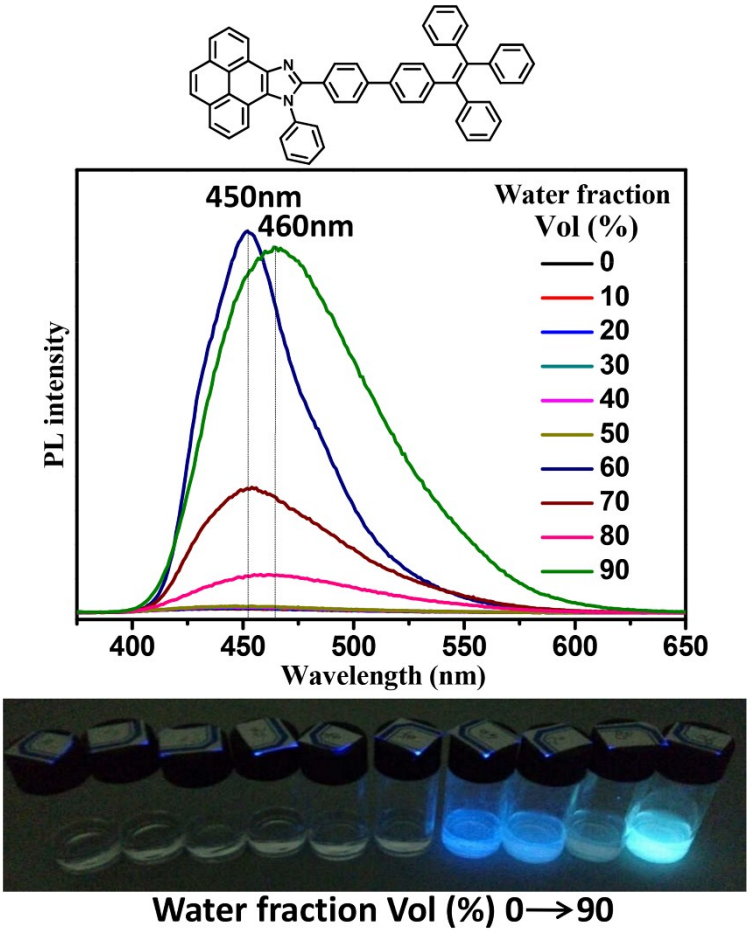


Fig. S11 Molecular structural formula of PyPTPEI and PL spectra in THF/water mixtures with different water fractions (f_w) and photograph in THF–water mixtures with different water fractions (f_w) under 365 nm UV illumination.

IV. Stacking mode, intermolecular interactions and structure refinements of crystals.

The CCDC number 1435680 contains the supplementary crystallographic data for PyTPEI.

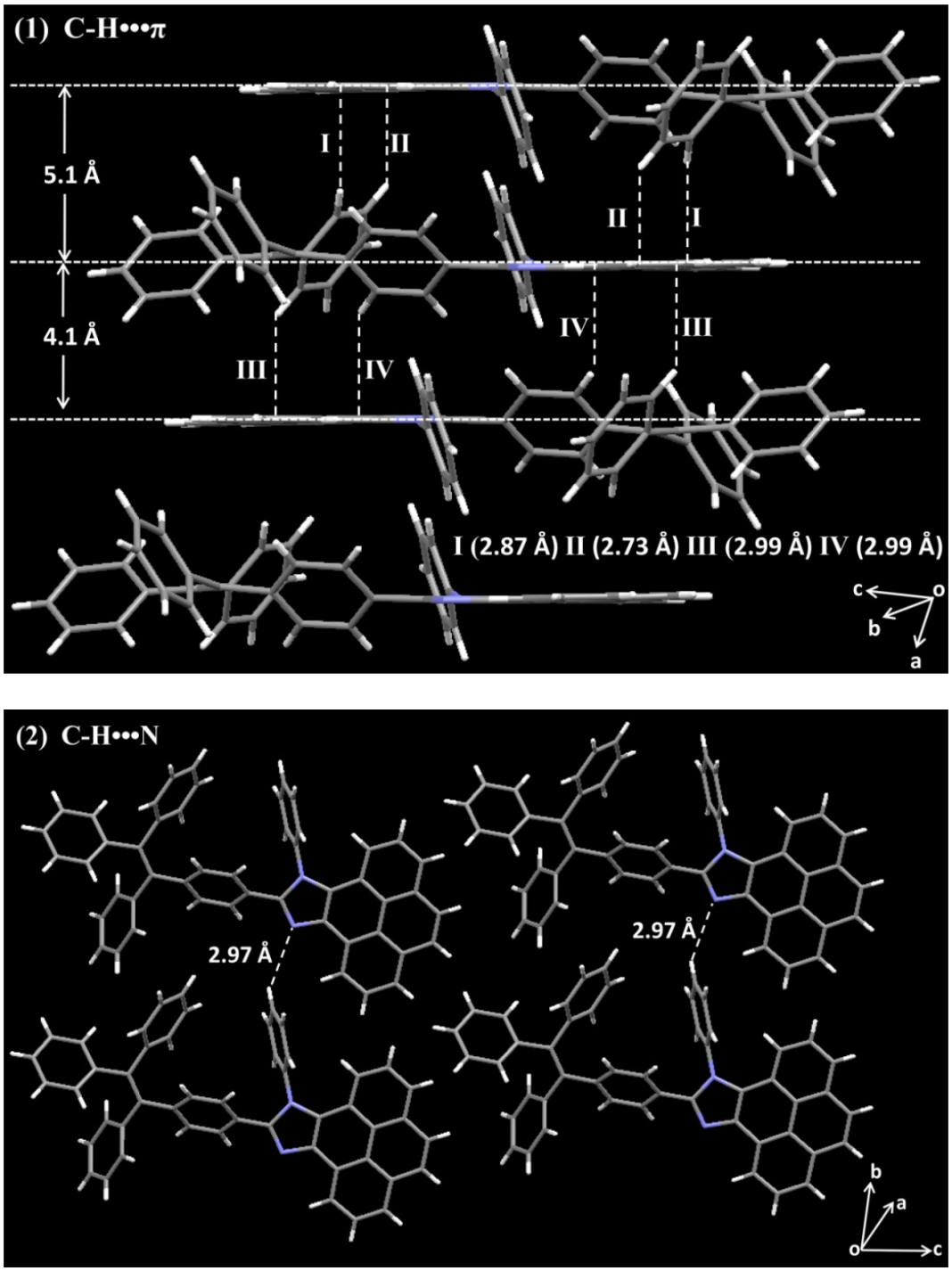


Fig. S12 Packing form and the intermolecular interactions including (1) C-H•••π (I, II, III, IV) and (2) C-H•••N (V) in PyTPEI crystal.

Table S1. Crystal data and structure refinement for PyTPEI.

	PyTPEI
empirical formula	$C_{49}H_{32}N_2$
formula wt	648.77
T, K	293(2)
crystal system	Triclinic
space group	P -1
a, Å	9.4323(19)
b, Å	9.962(2)
c, Å	18.769(4)
α,deg	83.37(3)
β,deg	81.36(3)
γ,deg	79.00(3)
V,Å^3	1404.7(6)
Z	2
density, Mg/m^3	1.264
Absorption coefficient, mm^{-1}	0.073
θ range, deg	3.15-27.48
no. of reflections collected	16799
no. of unique reflections	7711
R(int)	0.0406
Good-of-fit on F^2	1.093
R1 [$I > 2\sigma(I)$]	0.0599
wR2 [$I > 2\sigma(I)$]	0.1792
R1 (all data)	0.1069
wR2 (all data)	0.2051

V. Result of cyclic voltammetry measurement.

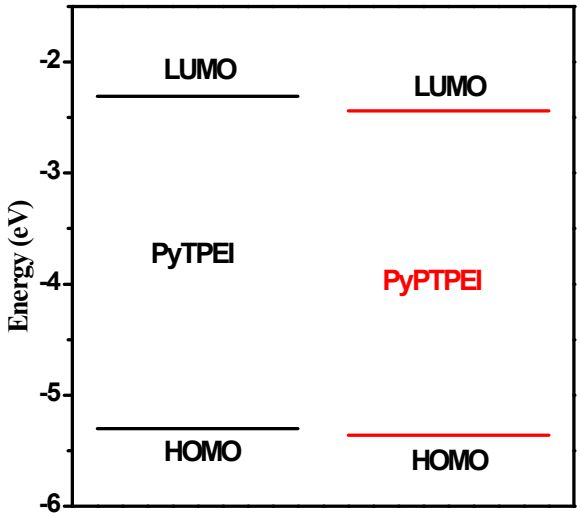


Fig. S13 HOMO-LUMO energy gaps obtained from CV measurement.

Table S2. Parameters of cyclic voltammograms for PyTPEI and PyPTPEI.

	E^{ox}_{onset} (V)[a]	E^{red}_{onset} (V)[a]	HOMO (eV)	LUMO (eV)	E_{gap} (eV)[b]
PyTPEI	**0.74**	**-2.25**	**-5.30**	**-2.31**	**2.99**
PyPTPEI	**0.80**	**-2.29**	**-5.36**	**-2.44**	**2.92**

[a] The initial oxidation and reduction potential. [b] Electrochemical bandgap.

VI. Optimization of molecular configuration and the dipole moment in ground state

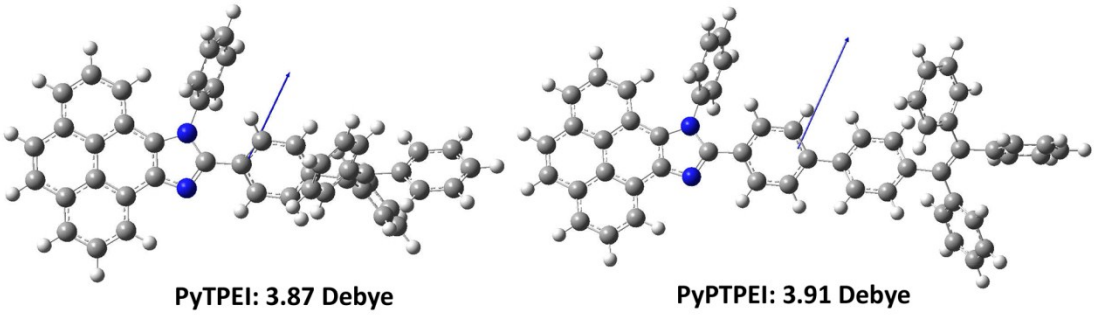


Fig. S14 Optimization of molecular configuration and the dipole moment in ground state on the basis of DFT results at the B3LYP/6-31G(d,p) level.

VII X-ray diffraction pattern of evaporated film.

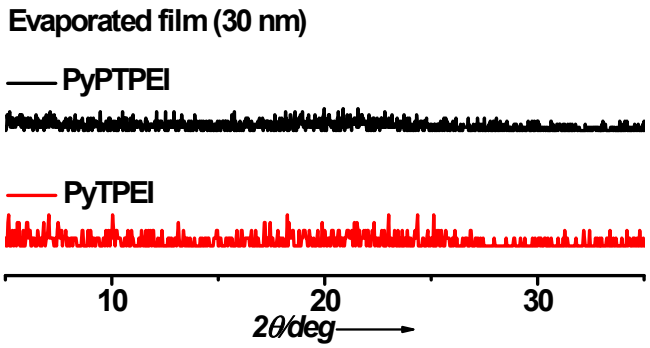


Fig. S15 XRD patterns of the original evaporated films for PyTPEI and PyPTPEI.