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Utilization of phenanthroimidazole based fluorophore in light emitting electrochemical cells

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UV-vis absorption and Photoluminescence spectra: The solution absorption and photoluminescence (PL) spectra of PYPN were measured in dilute THF solutions (Fig. S3 (d)). PL emission of PYPN in solution was centered on 458 nm. All the thin films used for PL measurements were prepared by spin casting corresponding dilute solutions onto glass substrate. The ratio of materials as well as solvents used were same as that of device manufacturing procedure. All the annealing processes were done at 120 °C for 1 h under vacuum. Solution spectra recorded with different components used in the active layer of LEC shows similar emission peak centered on 466 nm (Fig. 3 (d)), which is 8 nm red shifted from the PL spectra of PYPN in dilute THF solution. This slight red shift was later confirmed to be originated from using a mixture of solvents (THF and cyclohexanone). As-spun thin film photoluminescence spectra of PYPN (Fig. 3 (a)) shows a 19 nm red shift from its solution state (458 nm) to give a peak emission at 476 nm. The same after annealing exhibited a peak luminescence at 479 nm, slightly red shifted (3 nm) from its unannealed state. Both of the peak characteristics indicate that the red shift may be due to aggregation of PYPN in solid state or solvent effect. As-spun film containing PYPN, PEO and $LiCF_3SO_3$ (same ratio used for preparing active layer for device) exhibited an emission maximum at 509 nm (Fig. S1 (b)), which is further red shifted from unannealed PYPN film. On the other hand, annealed film of the same exhibited a peak at 526 nm, which is slightly red shifted from its device emission maxima by 5 nm. As-spun film containing PYPN and PEO exhibited an emission luminescence identical to the as-spun PYPN film. The corresponding film after annealing shows bad morphology due to strong phase separation and its emission peak was blue shifted by 9 nm from its unannealed state. In order to make sure the bathochromic shift was merely due the presence of ions, we prepared a film containing PYPN and $LiCF_3SO_3$ alone (Fig. S1 (c)). Unannealed film showed an emission peak at 472 nm with a shoulder on its right, indicating two types of emission, initial peak maxima corresponds to its solvated state by neutral solvent molecules in its thin film and shoulder may be from its ion interacted state. The corresponding annealed film emission was just like a mirror image of its as-spun film emission with a maximum at 522 nm similar to its electroluminescence peak and shoulder on its left corresponds to PYPN alone. The PL quantum yield of annealed film containing PYPN and lithium triflate shows a decrease in quantum yield, which is calculated to be 0.21 vs standard. The whole thin film measurements suggesting the strong bathochromic shift of EL may originate from PYPN-ion interactions.

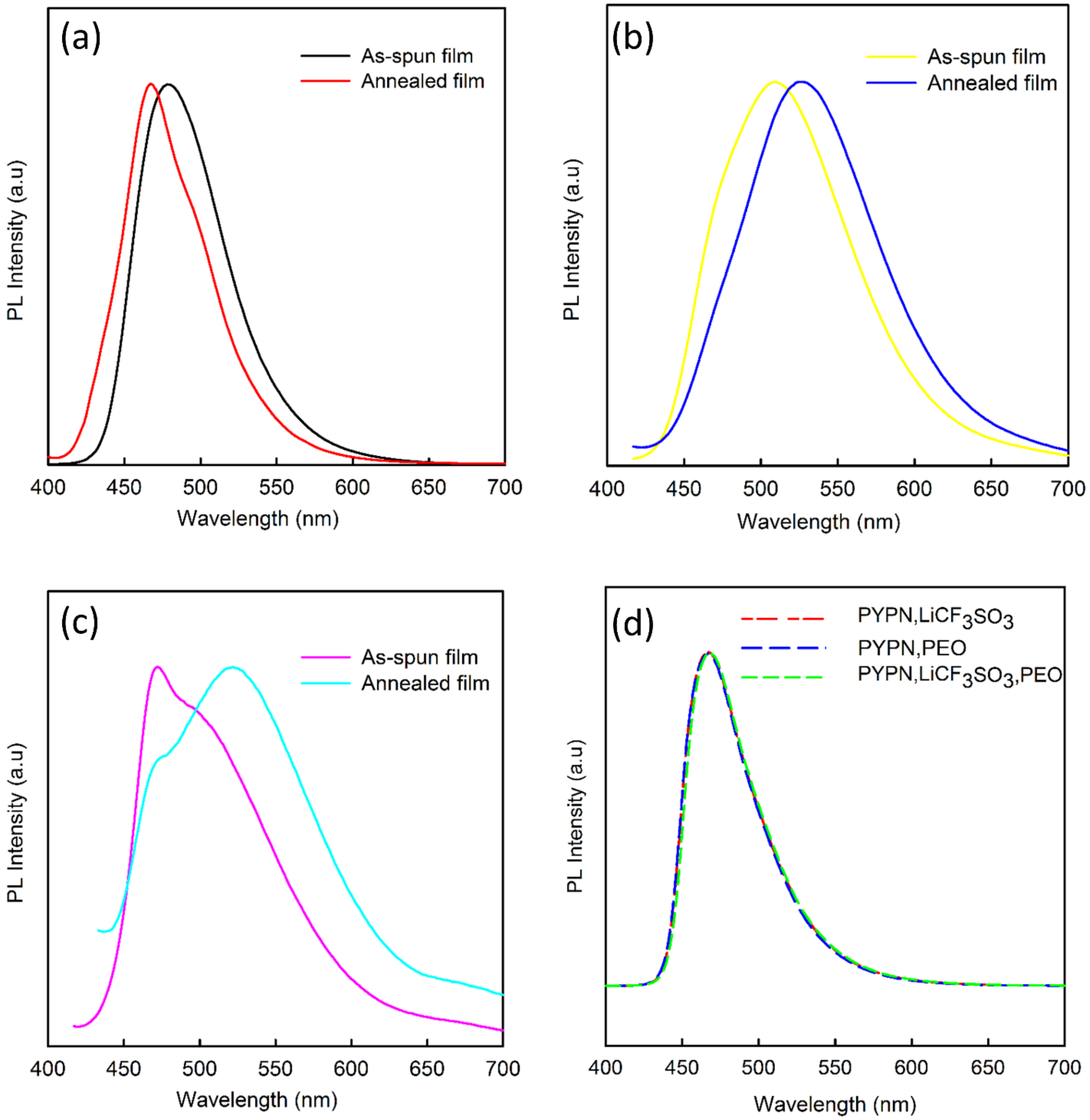

Figure S1. (a) PL spectra of PYPN and PEO thin film. (b) Thin film containing PYPN, PEO and $LiCF_3SO_3$ (c) Thin film containing PYPN and $LiCF_3SO_3$. (d) PL spectra in solution containing different components.

Table S1. Crystal data and structure refinement for PYPN.

CCDC	1041210	
Empirical formula	$C_{31}H_{18}N_2$	
Formula weight	418.47	
Temperature	173 (2) K	
Wavelength	0.71073 Å	
Crystal system	Rhombohedral	
Space group	R-3	
Unit cell dimensions	a = 24.4661(10) Å	α = 90°
	b = 24.4661(10) Å	β = 90°
	c = 20.545(2) Å	γ = 120°
Volume	10650.6(14) $Å^3$	
Z	18	
Density (calculated)	1.174 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F (000)	3924	
Crystal size	0.21 x 0.20 x 0.18 mm^3	
Theta range for data collection	1.38 to 26.00°.	
Index ranges	-30<=h<=26, -25<=k<=30, -25<=l<=25	
Reflections collected	17254	
Independent reflections	4637 [R (int) = 0.0684]	
Completeness to theta = 26.00°	99.60 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9877 and 0.9857	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4637 / 0 / 298	
Goodness-of-fit on F2	1.04	
Final R indices [I>2sigma (I)]	R1 = 0.0735, wR2 = 0.1903	
R indices (all data)	R1 = 0.1547, wR2 = 0.2145	
Largest diff. peak and hole	0.240 and -0.218 e. $Å^{-3}$	

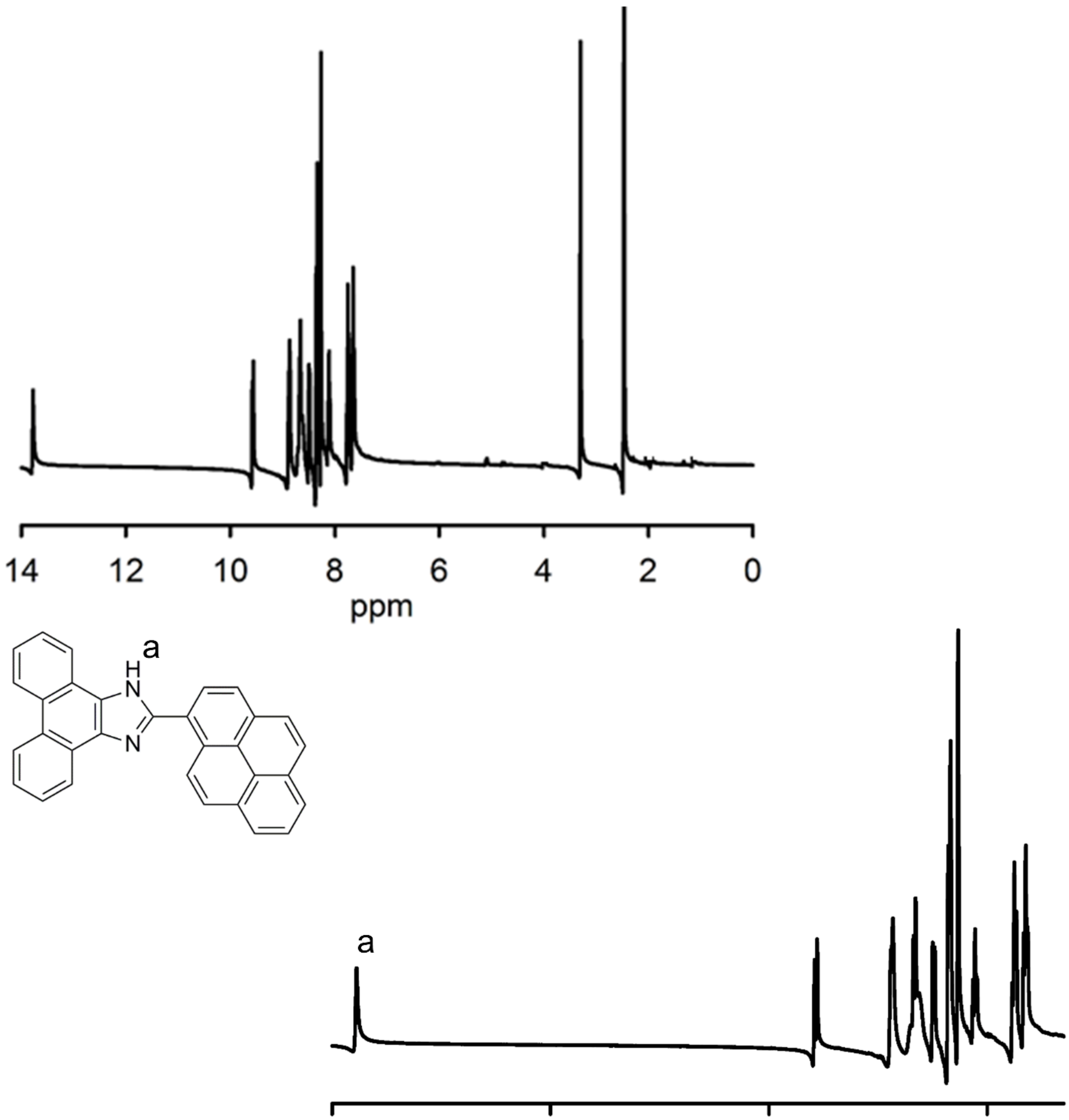

Figure S2. ^{1}H NMR Spectra of PYPN

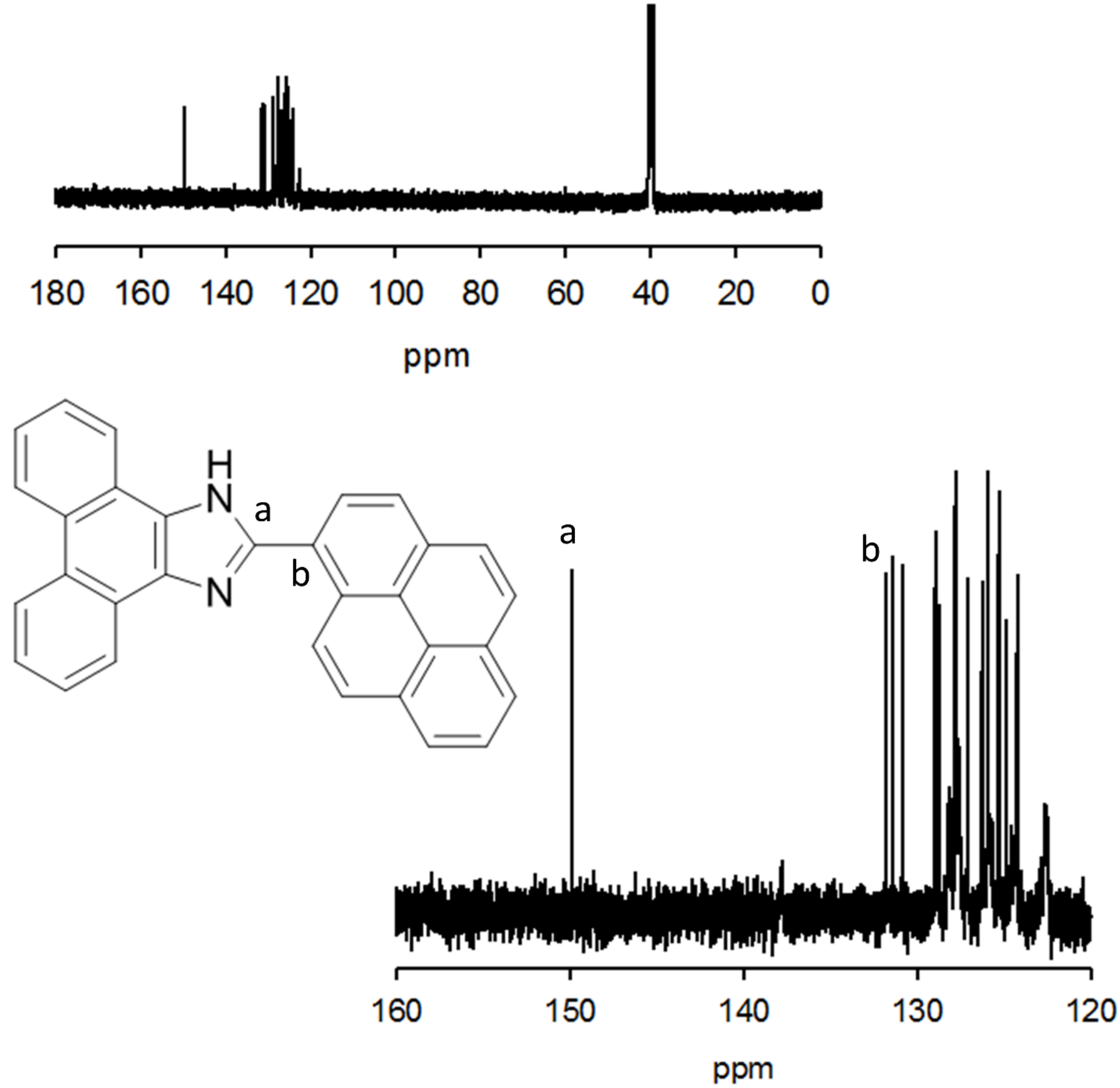

Figure S3. ^{13}C NMR Spectra of PYPN

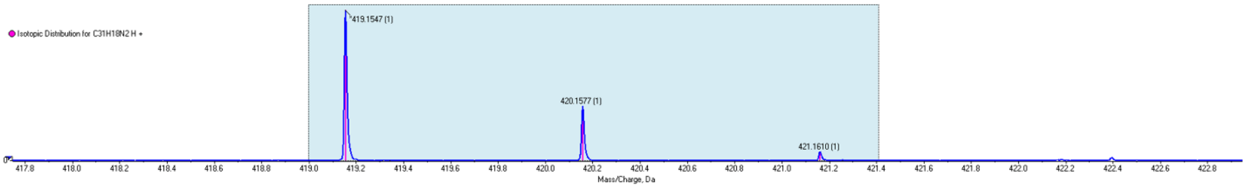

Figure S4. Mass Spectra of PYPN