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

Supporting Information

AIE-active 9,10-Bis(alkylarylvinyl)anthracences with Pendent Diethoxylphos-Phorylmethyl Groups as Solution-Processable Efficient EL Luminophore

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Supporting Materials, Methods and Figures

(1) ^{1}H NMR and ^{13}C NMR spectrums of PAC8 in $CDCl_3$

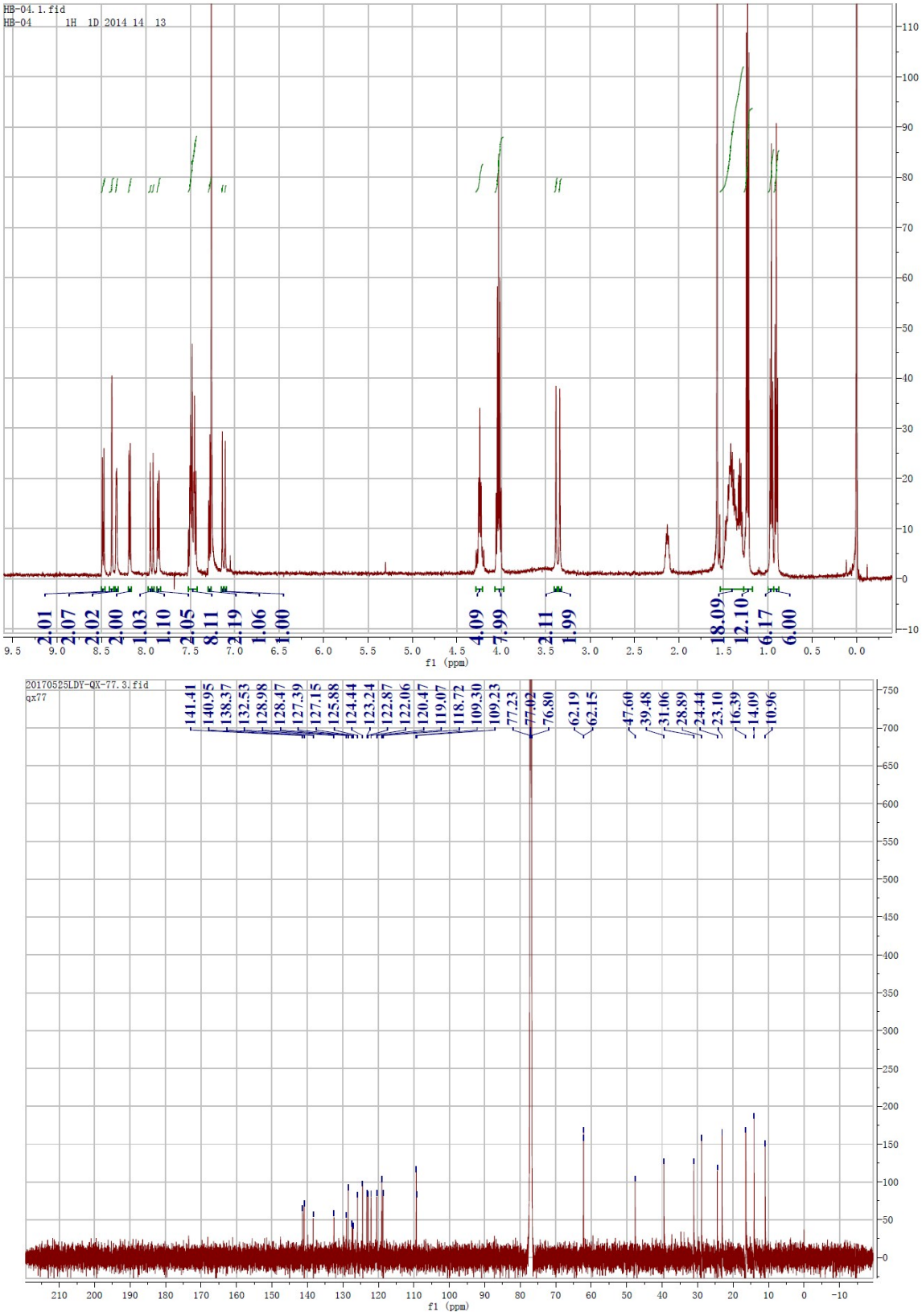

Figure S. ^{1}H NMR and ^{13}C NMR spectrums of PAC8 in $CDCl_3$.

(2) ^{1}H NMR and ^{13}C NMR spectrums of AC8 in $CDCl_3$

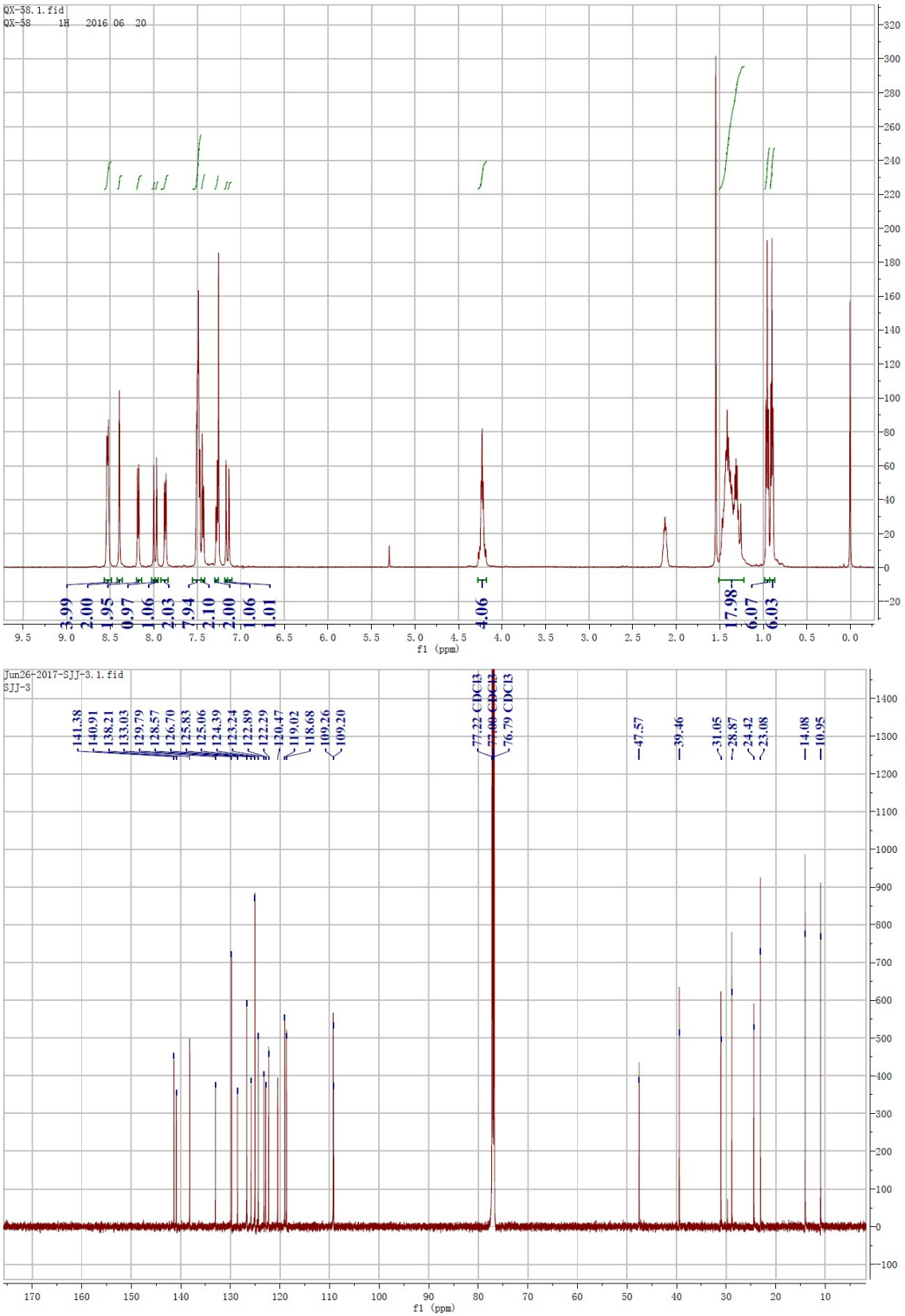

Figure S. ^{1}H NMR and ^{13}C NMR spectrums of AC8 in $CDCl_3$.

(3) Electronic structure and electrochemical properties

To gain a insight into the electronic structure, the spatial distributions of HOMO and LUMO of PAC8 were calculated with the density function theory (DFT) method with a B3LYP/6-31G(d) basis set using the Gaussian 09 package under the optimized molecular structure. The HOMO located on the phenylvinylanthracene moiety and N atoms, and the LUMO separated on anthracenevinyl unit. This implied that carbazole has played an electron-donating role, and the absorption and emission process may mainly be attributed to the π–π* transition along the conjugation backbone.

To evaluate the energy levels of the luminogen, the electrochemical properties were investigated by cyclic voltammetry (CV) in dichloromethane solution with 0.1 M tetrabutylammonium hexafluorophosphate as the supporting electrolyte at a scan rate of 100 mV/s using platinum as the working electrode and saturated calomel electrode as the reference electrode. The PAC8 exhibits a quasi-reversible oxidation process, with an onset potential at 0.37 V. which implies that the incorporation of the group can remarkably decrease the oxidation potential of the luminogen. The energy levels of HOMO [HOMO = (4.4 + E_{onset})] and LUMO [LUMO = HOMO + E_g] are thus determined by the onset potential of oxidation (E_{onset}) and the optical band gap. The HOMO energy level is calculated to be -5.63 eV. The quite similar HOMO energy level to that of PEDOT:PSS (-5.2 eV) indicates that hole injection is favored from PEDOT:PSS to the luminogen. The LUMO energy level is lower than that of 1,3,5-tris(*N*-phenylbenzimidazol-2-yl)benzene (TPBi, -2.7 eV), which may facilitate electron transporting in the emitting layer.

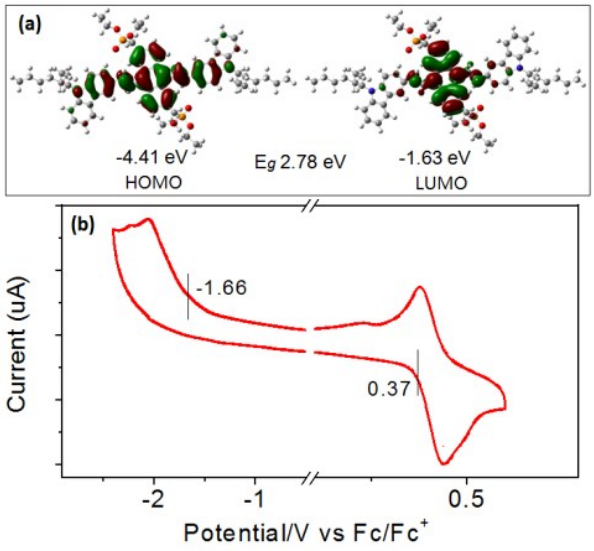

Figure S1 The density function theory (a) and cyclic voltammetry (b).

(4) The method of measuring/calculating external quantum efficiency (EQE)

The measured parameters included luminance, current and EL spectrum. EQE was calculated according to the formula below:

$$EQE = \frac{\pi \cdot L \cdot e}{683 \cdot I \cdot h \cdot c} \cdot \frac{\int_{380}^{780} I(\lambda) \cdot \lambda d\lambda}{\int_{380}^{780} I(\lambda) \cdot K(\lambda) d\lambda}$$

where L (cd m^{-2}) is the total luminance of device, I (A) is the current flowing into the EL device, λ (nm) is EL wavelength, I(λ) is the relative EL intensity at each wavelength and obtained by measuring the EL spectrum, K(λ) is the Commision International de L'Eclairage chromaticity (CIE) standard photopic efficiency function, e is the charge of an electron, h is the Planck's constant, c is the velocity of light.

(5) The spectral stability of the device based on PAC8 at different voltages.

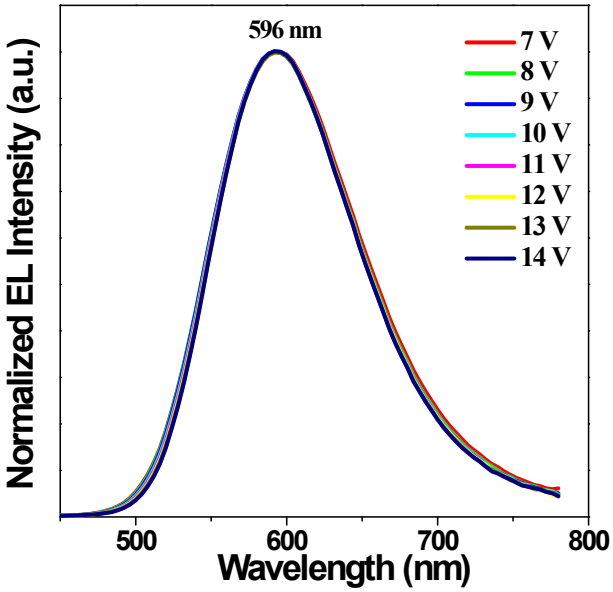

Figure S2 The spectra of the device at different voltages.