Electronic Supplementary Information (ESI)

Pyridyl-substituted anthracene derivatives incorporating solid-state emission and charge transport property

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^{1}H NMR information of the trhee compounds.

1a, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, J = 4.7 Hz, 2H), 8.67 (s, 2H), 8.56 (s, 2H), 8.16 (q, J = 8.9 Hz, 5H), 7.95 (d, J = 7.9 Hz, 2H), 7.84 (t, J = 7.5 Hz, 2H), 7.30 (d, J = 4.7 Hz, 2H).

1b, ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (s, 2H), 8.68 (s, 2H), 8.57 (s, 2H), 8.27 (s, 2H), 8.19 (d, J = 8.7 Hz, 4H), 7.76 (d, J = 8.4 Hz, 2H), 7.56 (s, 2H).

1b, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, J = 5.7 Hz, 4H), 8.57 (s, 2H), 8.33 (s, 2H), 8.17 (d, J = 8.8 Hz, 2H), 7.79 (dd, J = 8.8, 1.4 Hz, 2H), 7.70 (d, J = 6.0 Hz, 4H).

Table S1. Crystal data and structure refinement of **1a**, **1b** and **1c**. (CCDC No. 1439492, 1439493, 1439496.)

Compound	**1a** (1439492)	**1b** (1439493)	**1c** (1439496)
Empirical formula	C24 H16 N2	C24 H16 N2	C24 H16 N2
Formula weight	332.39	332.39	332.39
Temperature	113(2) K	123(2) K	173.1500 K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Orthorhombic	Monoclinic
Space group	P2(1)/c	Pca2(1)	P 1 21/c 1
Unit cell dimensions	a = 17.318(4) Å b = 6.2349(12) Å c = 7.3422(15) Å a= 90° β= 96.81(3)° γ = 90°.	a = 7.4367(15) Å b = 6.2803(13) Å c = 35.030(7) Å a= 90° β= 90°, γ= 90°.	a = 12.582(10) Å b = 5.997(5)Å c = 10.882(9) Å a= 90° β= 103.308(13)° γ= 90°.
Volume	787.2(3) $Å^3$	1636.1(6) $Å^3$	799.1(11) $Å^3$
Z	2	4	2
Density (calculated)	1.402 Mg/m^3	1.349 Mg/m^3	1.381 Mg/m^3
Absorption coefficient	0.083 mm^{-1}	0.080 mm^{-1}	0.081 mm^{-1}
F(000)	348	696	348
Crystal size	0.20 x 0.18 x 0.12 mm^3	0.32 x 0.30 x 0.12 mm^3	0.39 x 0.37 x 0.03 mm^3
Theta range for data collection	2.37 to 27.95°	2.33 to 25.99°	3.328 to 27.397°
Index ranges	-22 ≤ h ≤ 22 -8 ≤ k ≤ 7 -9 ≤ l ≤ 9	-9 ≤ h ≤ 8 -7 ≤ k ≤ 7 -43 ≤ l ≤ 43	-16 ≤ h ≤ 15 -7 ≤ k ≤ 7 -14 ≤ l ≤ 14
Reflections collected	8756	8767	6164
Independent reflections	1882 [R(int) = 0.0402]	2986 [R(int) = 0.0819]	1810 [R(int) = 0.0553]
Max. and min. transmission	0.9902 and 0.9837	0.9905 and 0.9750	1.0000 and 0.6325
Data / restraints / parameters	1882/0/118	2986/1/236	1810 / 0 / 118
Goodness-of-fit on F2	1.063	0.997	1.194
Final R indices [I>2sigma(I)]	R1 = 0.0404 wR2 = 0.1091	R1 = 0.0816 wR2 = 0.1974	R1 = 0.0746 wR2 = 0.1722
R indices (all data)	R1 = 0.0497 wR2 = 0.1131	R1 = 0.1004 wR2 = 0.2145	R1 = 0.0825 wR2 = 0.1775
Largest diff. peak and hole	0.310 and -0.222 $e.Å^{-3}$	0.529 and -0.406 $e.Å^{-3}$	0.283 and -0.267 $e.Å^{-3}$

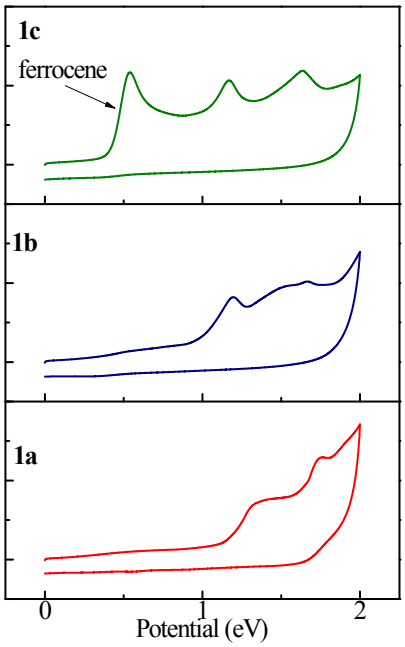

Figure S1. Cyclic voltammetry measurements of 1a-c with ferrocene as inner standard.

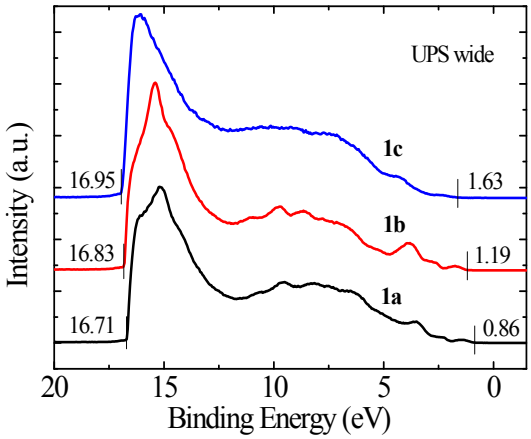

Figure S2. Ultraviolet photoelectron spectroscopy (UPS) measurements of 1**a-c**. The sample for UPS measurement was prepared by depositing a thin film (8 nm) on a small plate of ITO (size: 1 cm × 1 cm). The ionization potential was obtained using the formula $I=h-(E_K^{max}- E_K^{cut\text{-}off})$. The cut-off at the left-hand part of UPS (He I) energy distribution curves E_K^{max} corresponds to electrons that have just enough energy to escape from the solid to vacuum level and the maximum kinetic energy $E_K^{cut\text{-}off}$ at the right-hand part corresponds to electrons from the HOMO level.

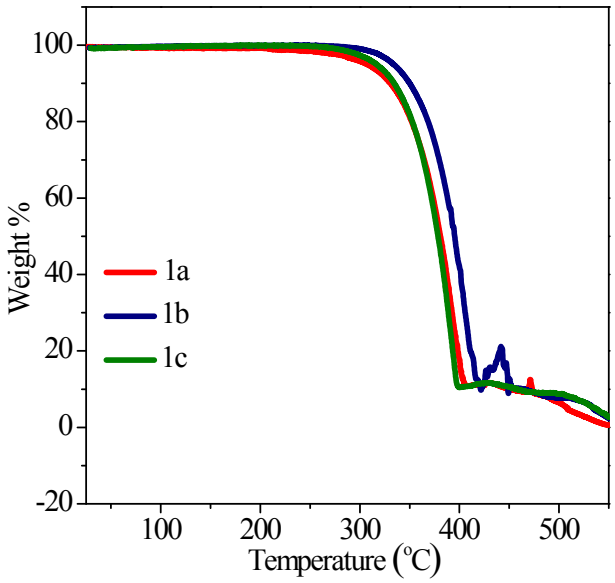

Figure S3. Thermogravimetric analysis of **1a**, **1b** and **1c**.

Table S3. Summary of absorption and emission characters and calculated band gaps, orbital energy levels and decomposition temperatures of **1a**, **1b** and **1c**.

	λ_{onset} (nm)	E_g (eV)	$\lambda_{0\text{-}0,Abs}$ (nm)	$\lambda_{0\text{-}0,PL}$ (nm)	HOMO[a] (eV)	HOMO[b] (eV)	T_{dec} (°C)
1a	420	2.95	407	417	-5.55	-5.37	307
1b	411	3.01	398	410	-5.4	-5.58	333
1c	421	2.95	403	420	-5.4	-5.9	316

[a] HOMO levels calculated from CV test, [b] HOMO levels obtained from UPS.

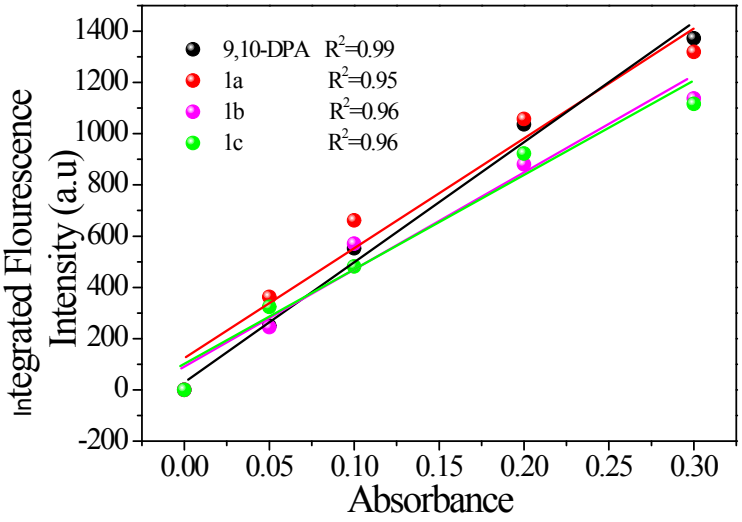

Figure S4. Fluorescence quantum efficiency of **1a**, **1b** and **1c** monomers. The efficiency of three compounds in solution were measured in comparison with 9,10-diphenyl anthracene (9,10-DPA). Cyclohexane (η=1.42662) was used as solvent for 9,10-DPA, and THF (η=1.4050) was used for the three compounds and the excite wavelength was fixed at 370 nm, ΦF of 90% was reported for 9,10-DPA, and the calculated ΦF of **1a**, **1b**, **1c** monomers was 86.0%, 75.2%, 73.7%, respectively.

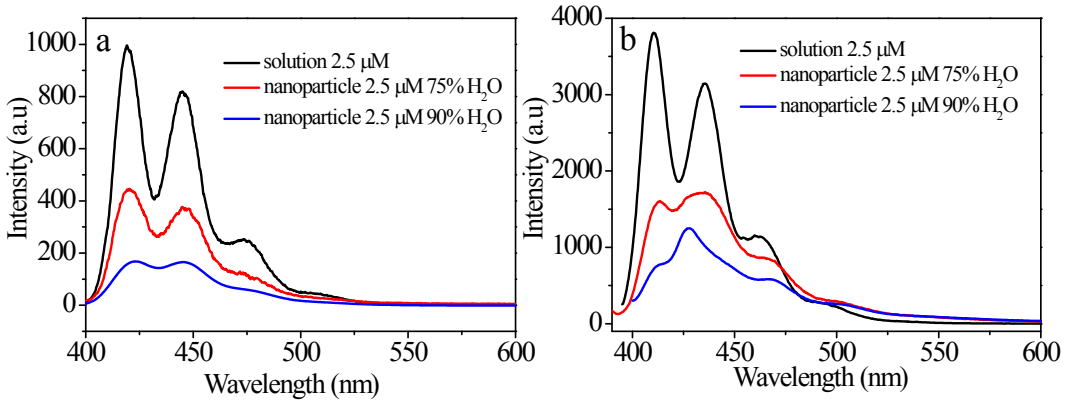

Figure S5. Evidence of aggregation caused quenching (ACQ) effect of **1a** (a) and **1b** (b).

Table S3. Criterions of H- and J-aggregates.

	Absorption	Relative Intensity of 0-0 peak	Stokes shift	Radiative deacay rate/k_f
H-aggregates	Blue-shifted	Decreased	Increased	Decreased
J-aggregates	Red-shifted	Increased	Decreased	Increased

By comparing nanoparticles with monomers, H-aggregates usually show blue-shifted absorption, decreased relative intensity of 0-0 peak, increased stokes shift and decreased radiative decay rate k_f, where $k_f = \Phi_F/\tau$.[1-3]

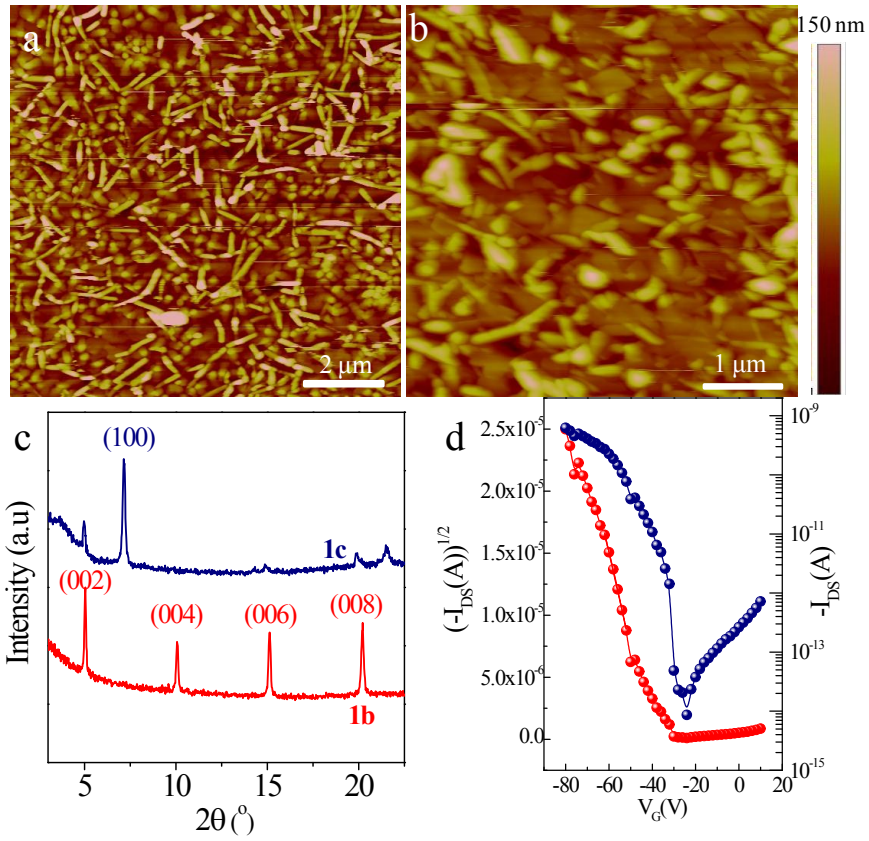

Figure S6. AFM (a, b) and XRD (c) characterization of 1b and 1c thin films; and typical transfer characteristics of thin film FETs based on **1b**. The output curve was unable to get because of the poor performance.

References

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2. Z. Xu, Q. Liao, Y. Wu, W. Ren, W. Li, L. Liu, S. Wang, Z. Gu, H. Zhang, H. Fu, *J. Mater. Chem.*, 2012, **22**, 17737-17743.
3. F. C. Spano, *Accounts Chem. Res.*, 2009, **43**, 429-439.