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Highly stable and efficient deep-red phosphorescent organic light-emitting devices using phenanthroline derivative as n-type exciplex host partner

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General Information

Quantum chemical calculations were performed using the hybrid density functional theory (DFT), functional Becke and Hartree-Fock exchange, and Lee Yang and Parr correlation (B3LYP) as implemented in the Gaussian 09 program packages.[1] Electrons were described by the Pople 6-31G(d,p) and 6-311+G(d,p) basis sets for molecular structure optimization and single-point energy calculations, respectively. Differential scanning calorimetry (DSC) was performed using a Perkin-Elmer Diamond DSC Pyris instrument under nitrogen atmosphere at a heating rate of 10°C min^{-1}. Thermogravimetric analysis (TGA) was undertaken using a SEIKO EXSTAR 6000 TG/DTA 6200 unit under nitrogen atmosphere at a heating rate of 10°C min^{-1}. UV-Vis spectra was measured using a Shimadzu UV-3150 UV-vis-NIR spectrophotometer. Photoluminescence spectra were measured using a FluroMax-2 (Jobin-Yvon-Spex) luminescence spectrometer. The ionization potential (I_p) was determined using a Sumitomo Heavy Industries, Ltd PYS-201 in vacuum (~10^{-3} Pa).[2] Photoluminescence quantum yield were measured using a Hamamatsu C11347 absolute PL quantum yield spectrometer with an integral sphere at an excitation wavelength of each sample. Atomic Force Microscope (AFM) images were obtained by Agilent 5000.

[1] *Gaussian 09*, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[2] H. Ishii, D. Tsunami, T. Suenaga, N. Sato, Y. Kimura, M. Niwano, *J. Surf. Sci. Soc. Jpn.* 2007, *28*, 264.

Device Fabrication

The substrates were cleaned with ultra-purified water and organic solvents, and then dry-cleaned for 20 minutes by exposure to UV–ozone. The organic layers were deposited onto the ITO substrates under the vacuum (=10^{-5} Pa), successively. Al was patterned using a shadow mask with an array of 2 mm × 2 mm openings without breaking the vacuum (=10^{-5} Pa). The electroluminescent (EL) were taken using an optical multichannel analyzer Hamamatsu Photonics PMA-11. The current density–voltage and luminance–voltage characteristics were measured by using a Keithley source measure unit 2400 and a Minolta CS2000 luminance meter, respectively.

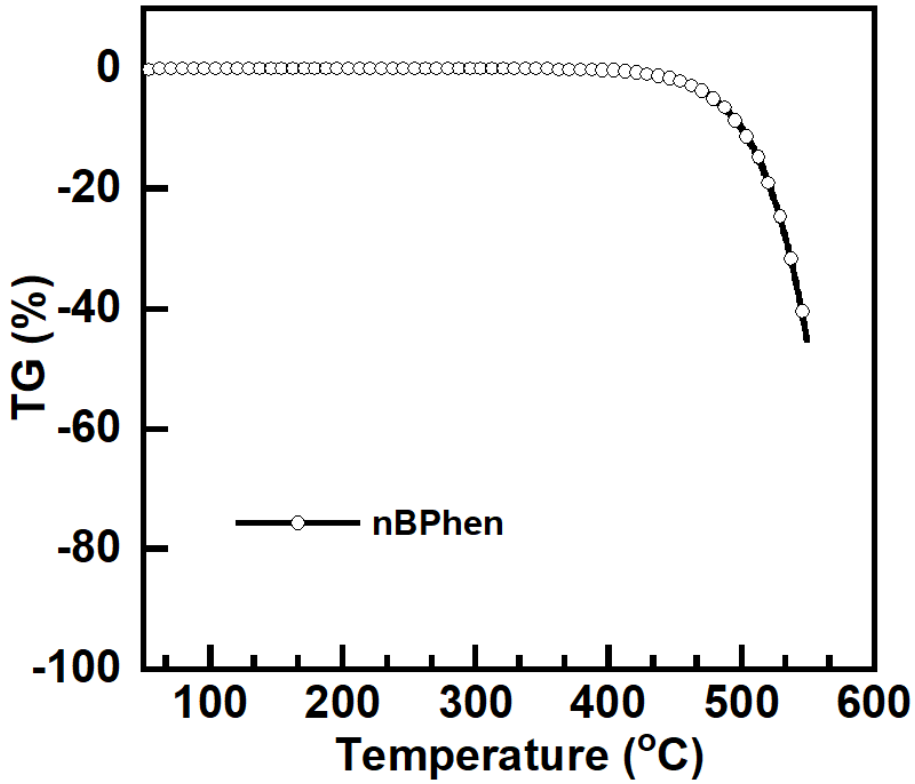

Figure S1 TGA thermogram of **nBPhen.**

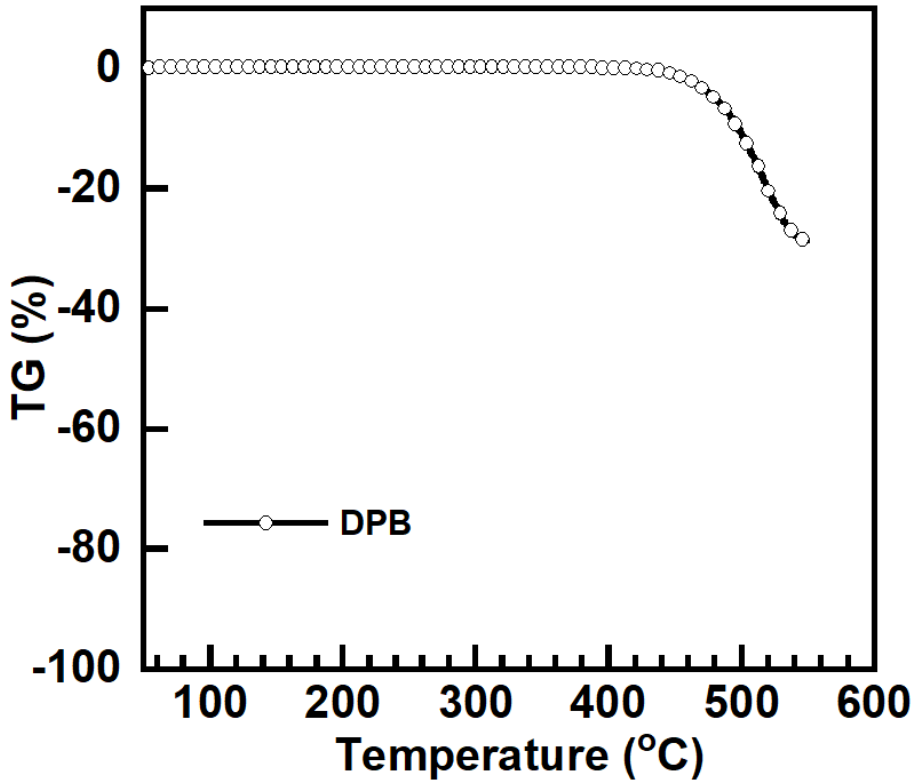

Figure S2 TGA thermogram of **DPB**.

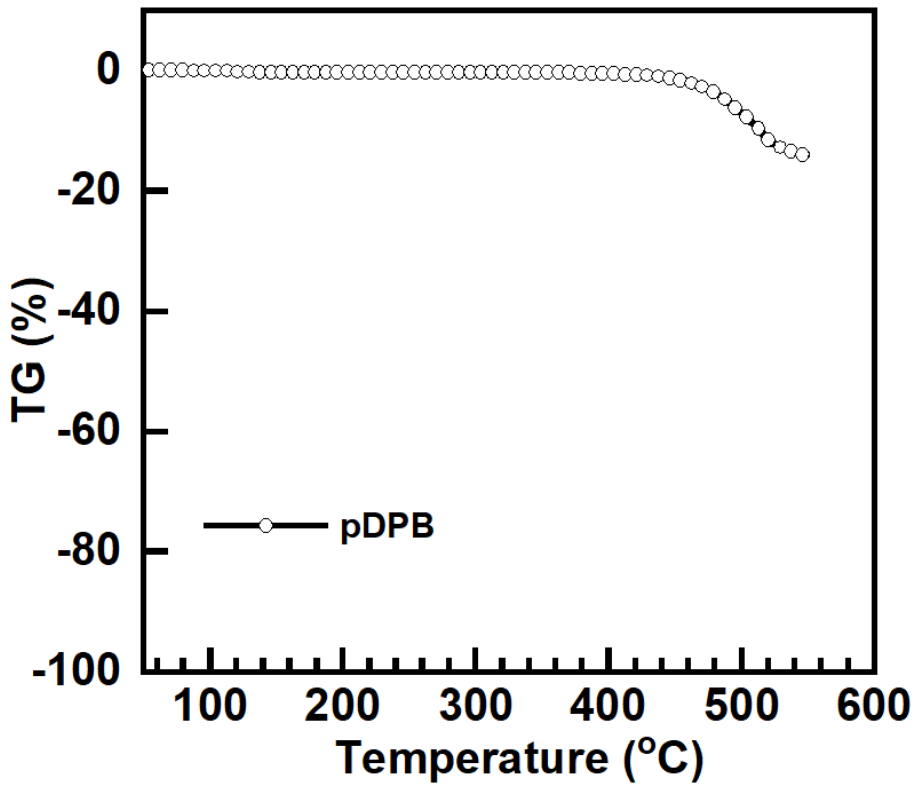

Figure S3 TGA thermogram of **pDPB**.

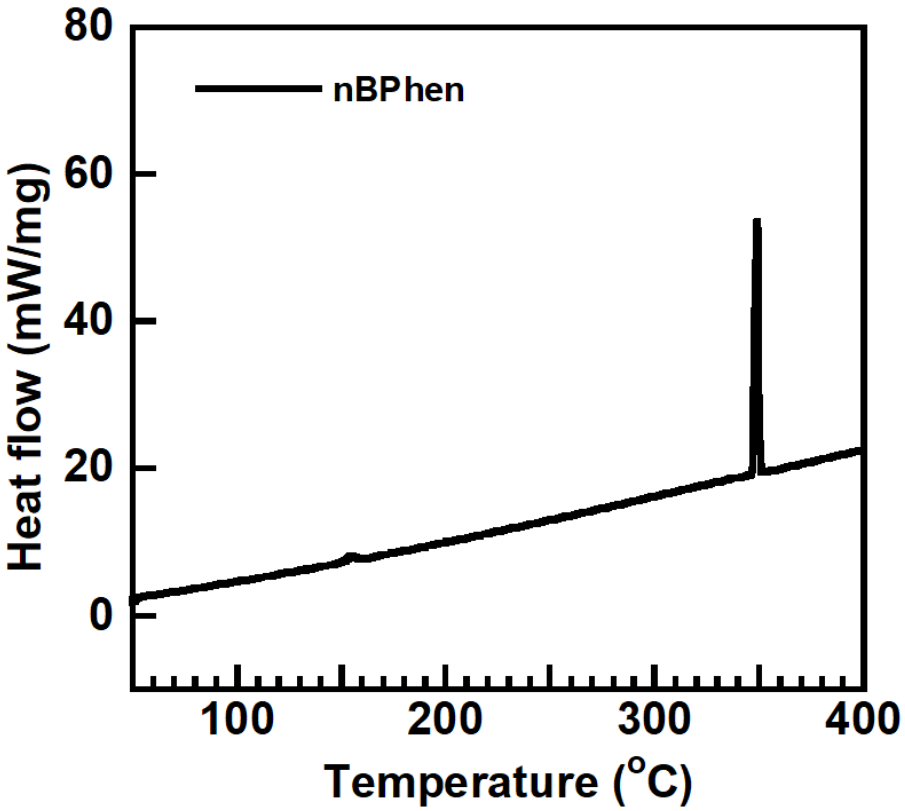

Figure S4 DSC curve of **nBPhen**.

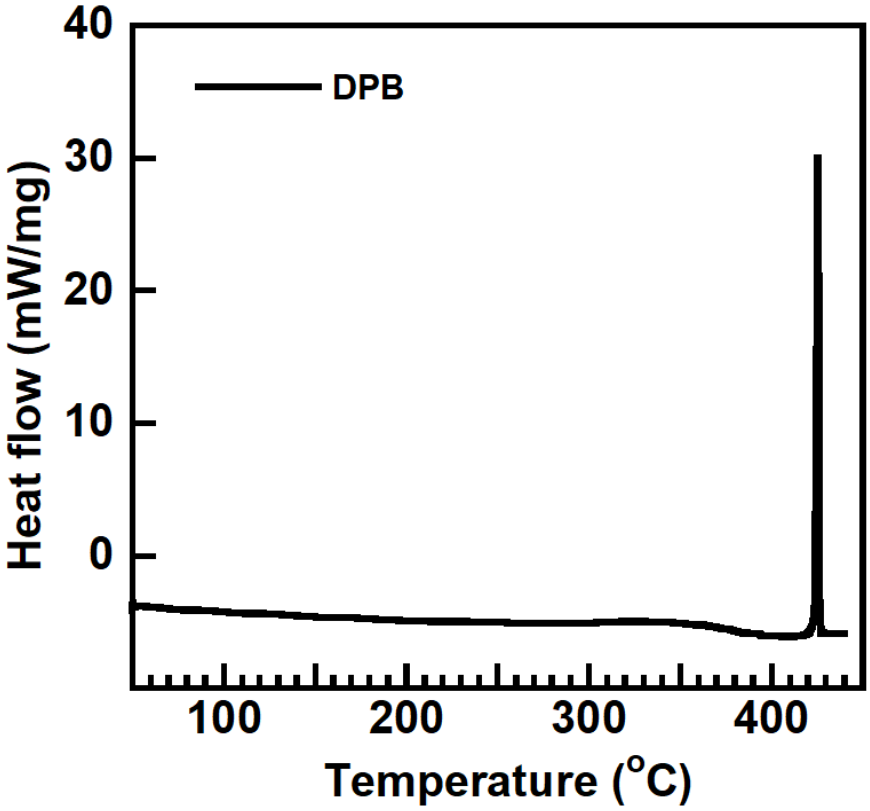

Figure S5 DSC curve of **DPB**.

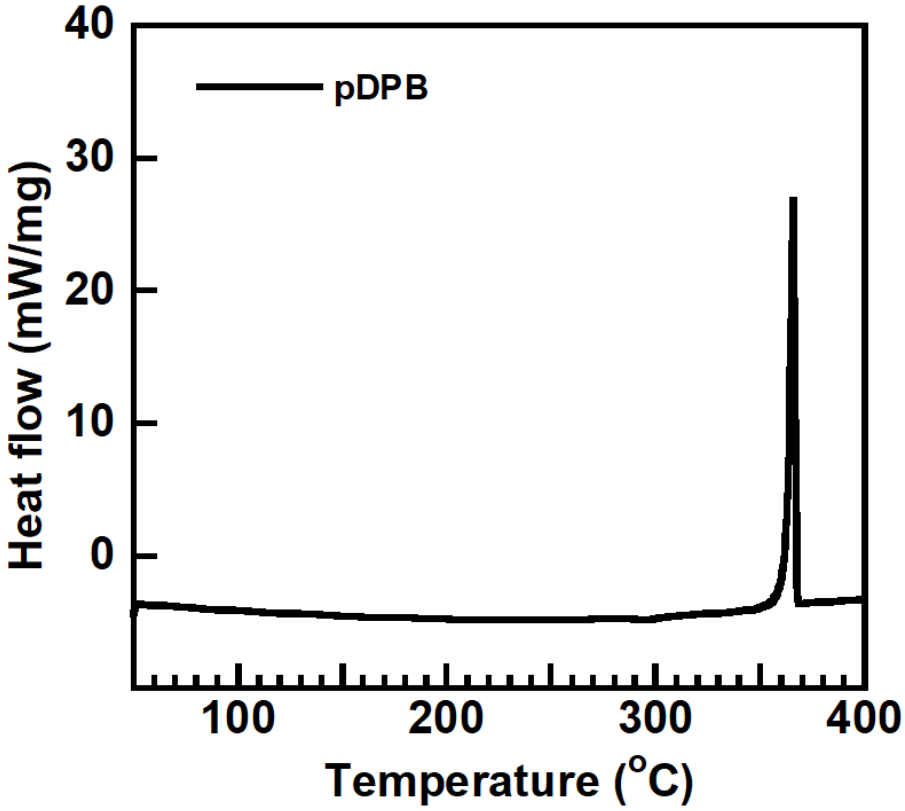

Figure S6 DSC curve of **pDPB**.

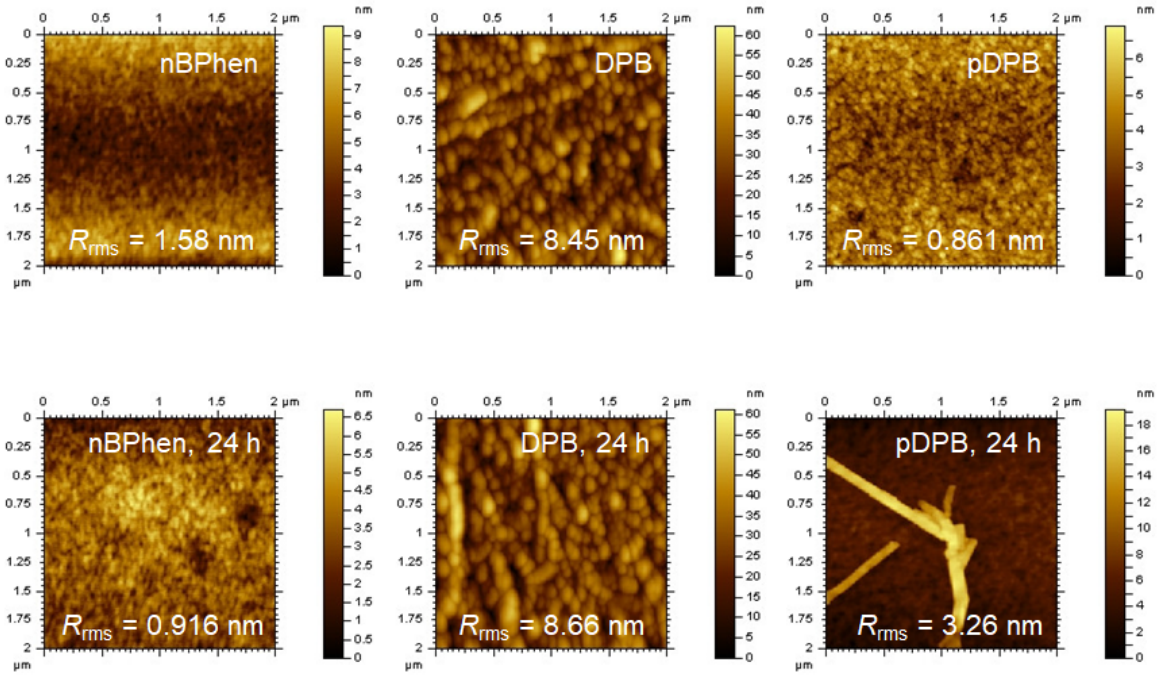

Figure S7 AFM images of **nBPhen**, **DPB** and **pDPB** films measured right after and 24 h after the film preparation.

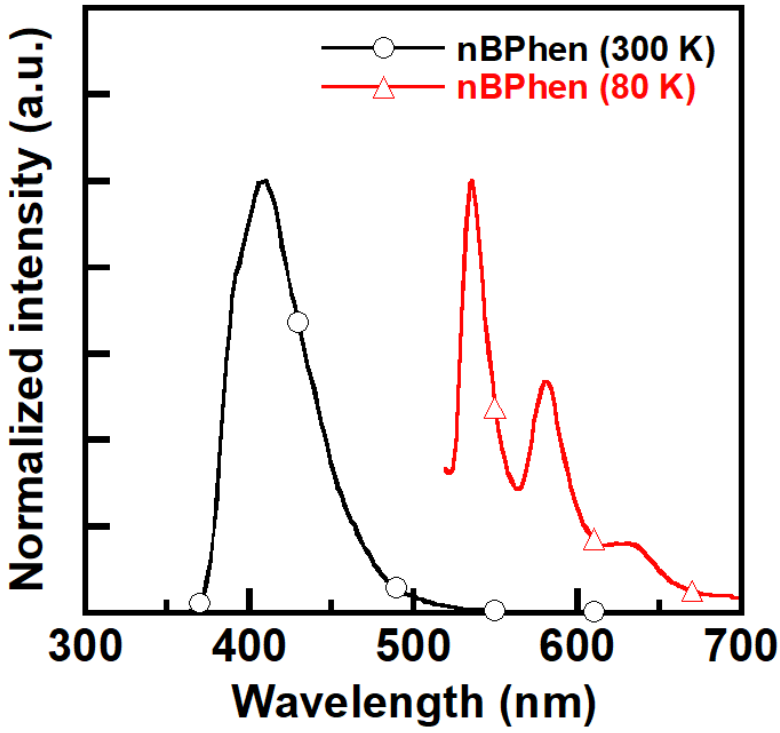

Figure S8 PL spectra in 2-methyltetrahydrofuran solution of **nBPhen** at 300 K (excited at 330 nm) and 80 K (excited at 380 nm).

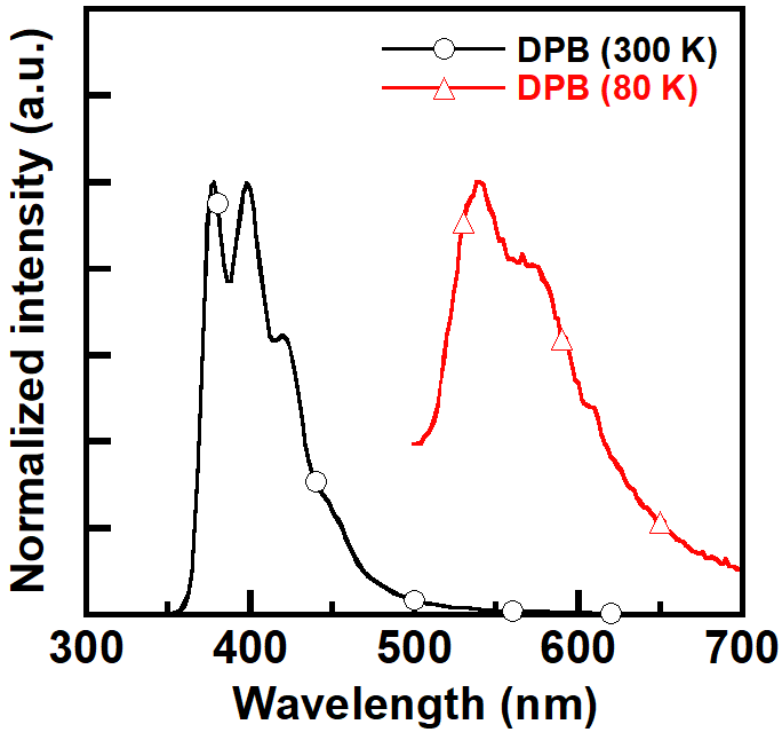

Figure S9 PL spectra in 2-methyltetrahydrofuran solution of **DPB** at 300 K (excited at 330 nm) and 80 K (excited at 450 nm).

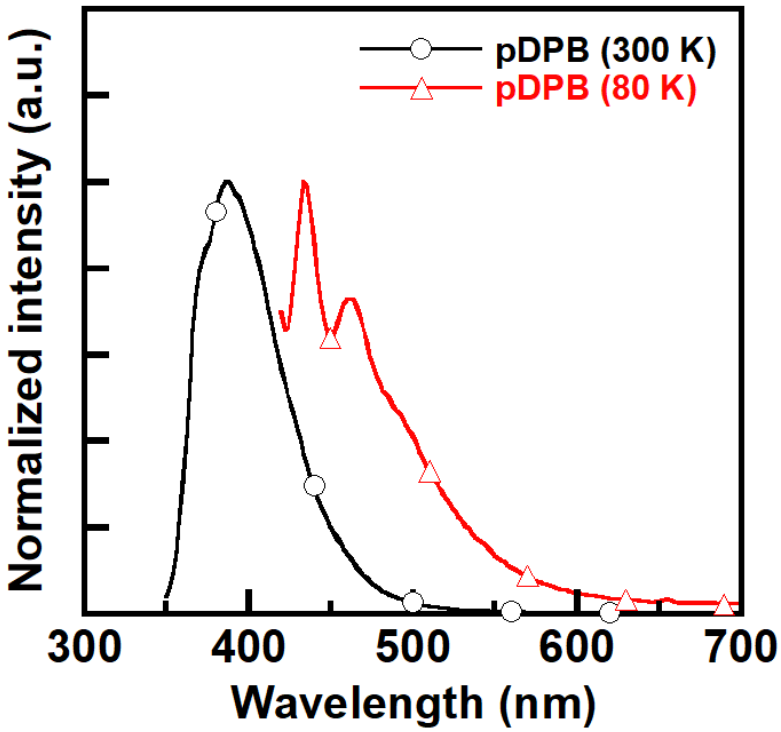

Figure S10 PL spectra in 2-methyltetrahydrofuran solution of **pDPB** at 300 K (excited at 330 nm), and toluene solution at 80 K (excited at 400 nm).

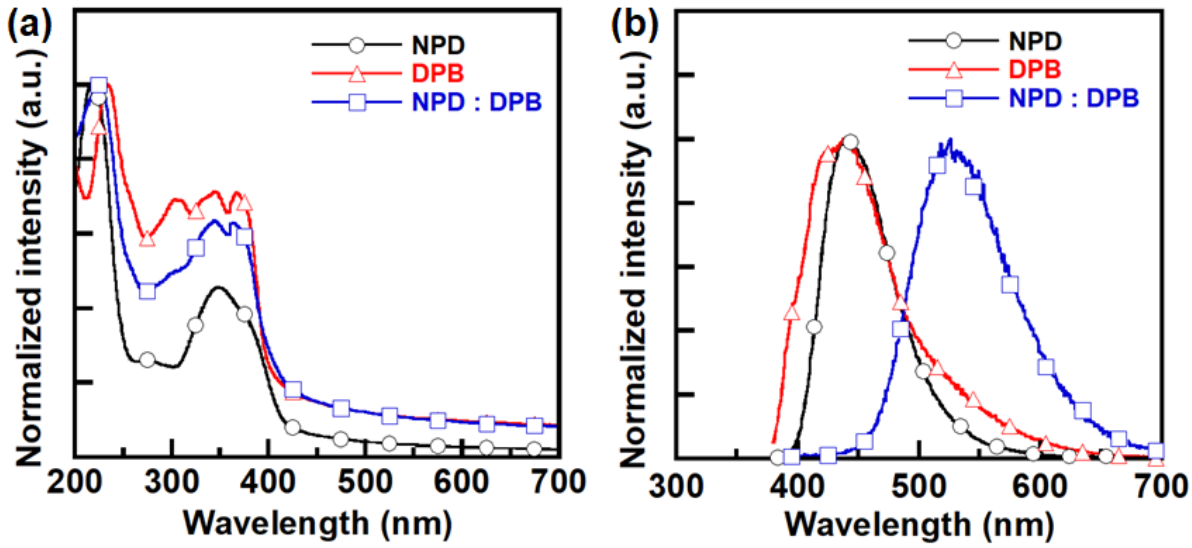

Figure S11 (a) Normalized UV-vis absorption and (b) normalized PL spectra of the **NPD**, **DPB** and **NPD : DPB** (1 : 1, molar ratio) co-deposited film.

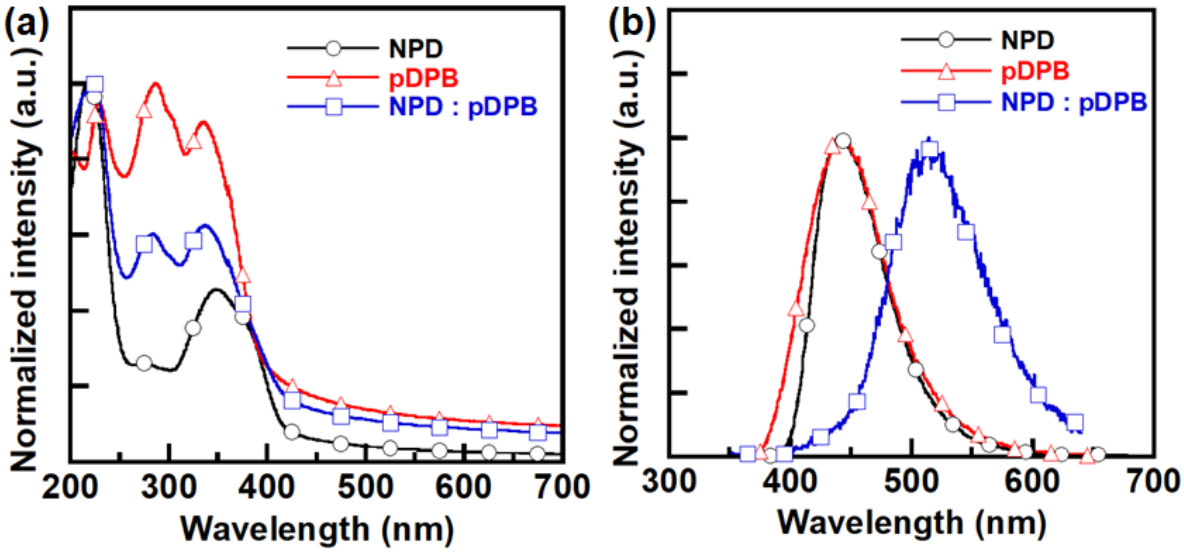

Figure S12 (a) Normalized UV-vis absorption and (b) normalized PL spectra of the **NPD**, **pDPB** and **NPD : pDPB** (1 : 1, molar ratio) co-deposited film.

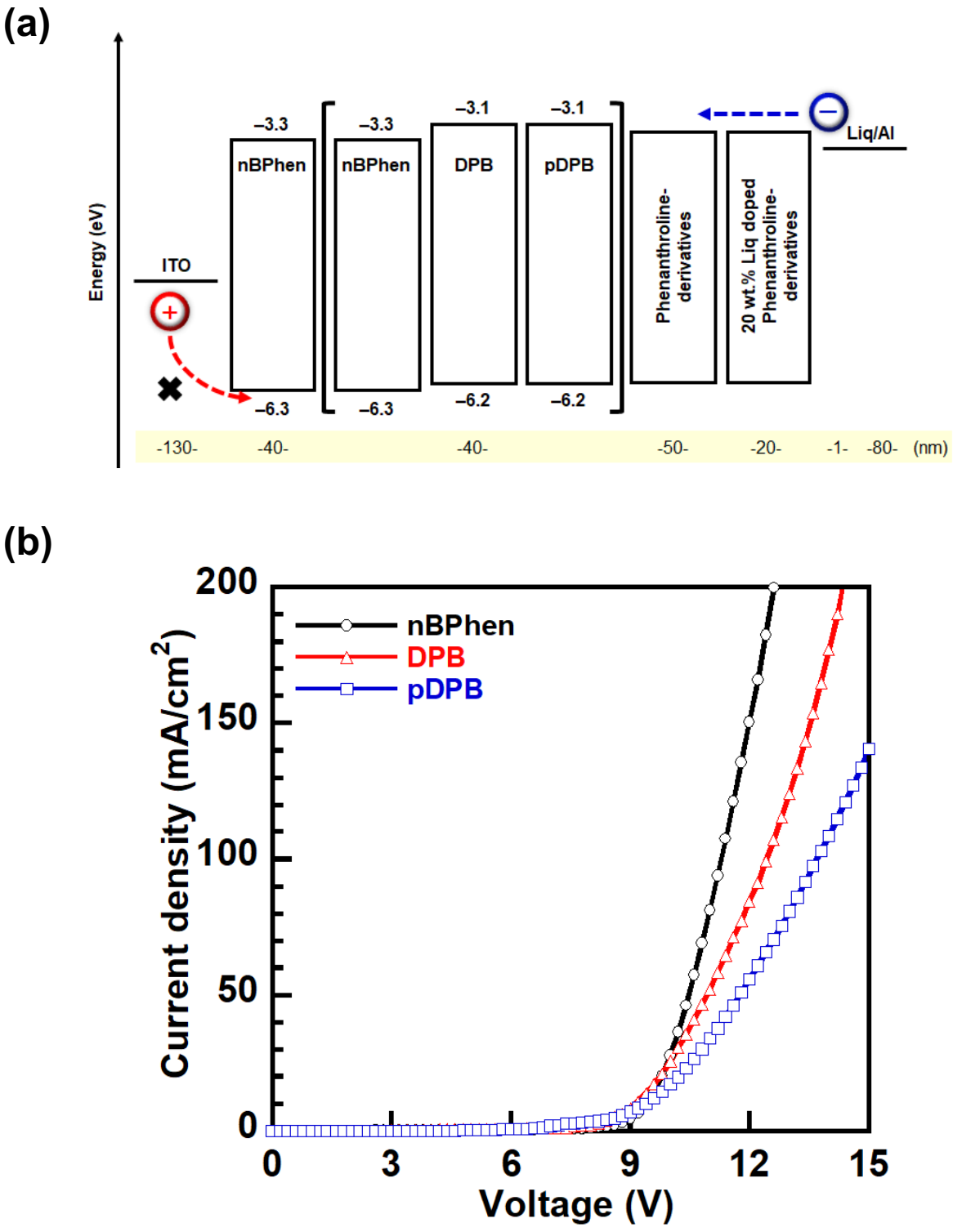

Figure S13. (a) Energy diagram, and (b) J-V characteristics of the electron-only devices without p-type host partner.

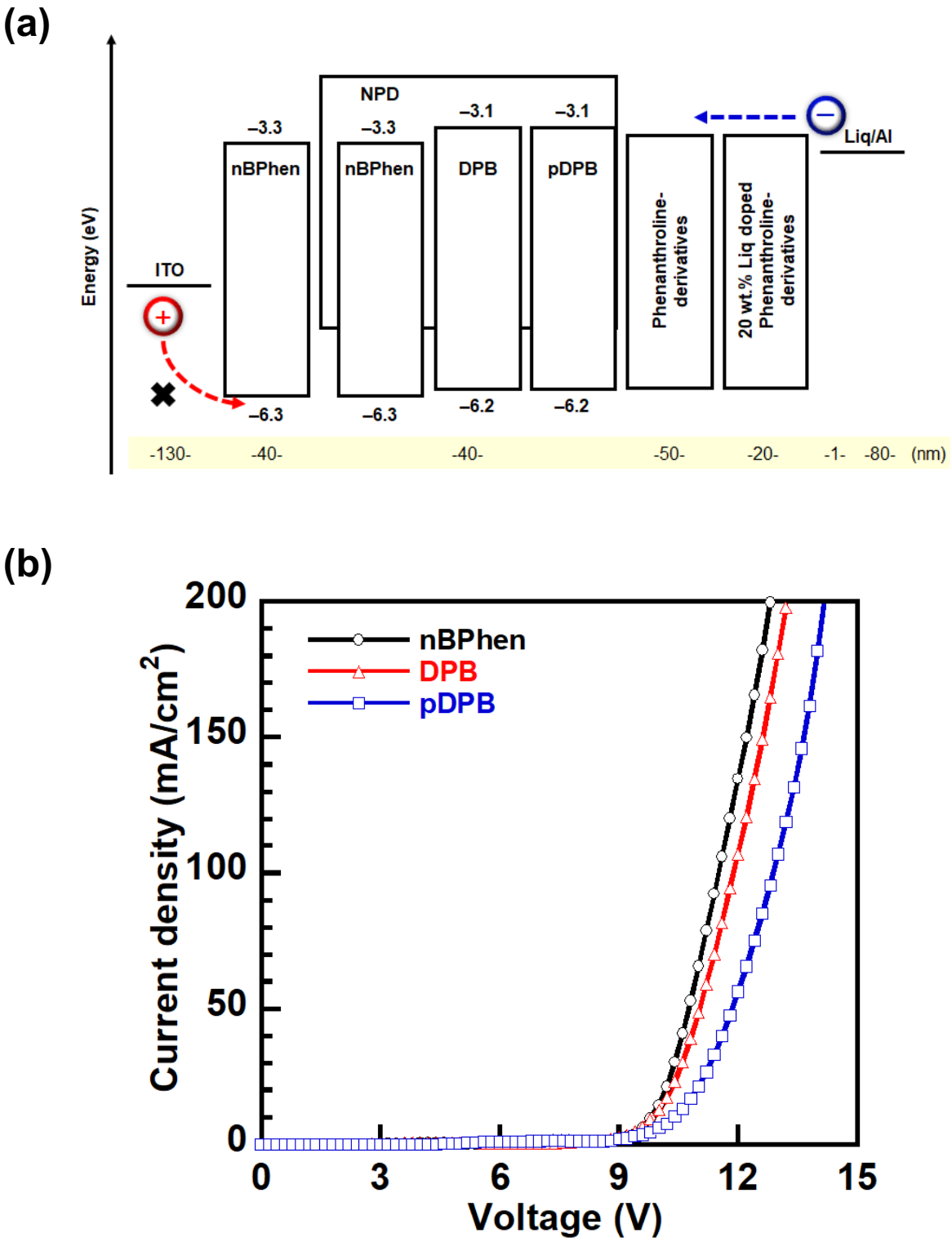

Figure S14. (a) Energy diagram, and (b) J-V characteristics of the electron-only devices with p-type host partner.

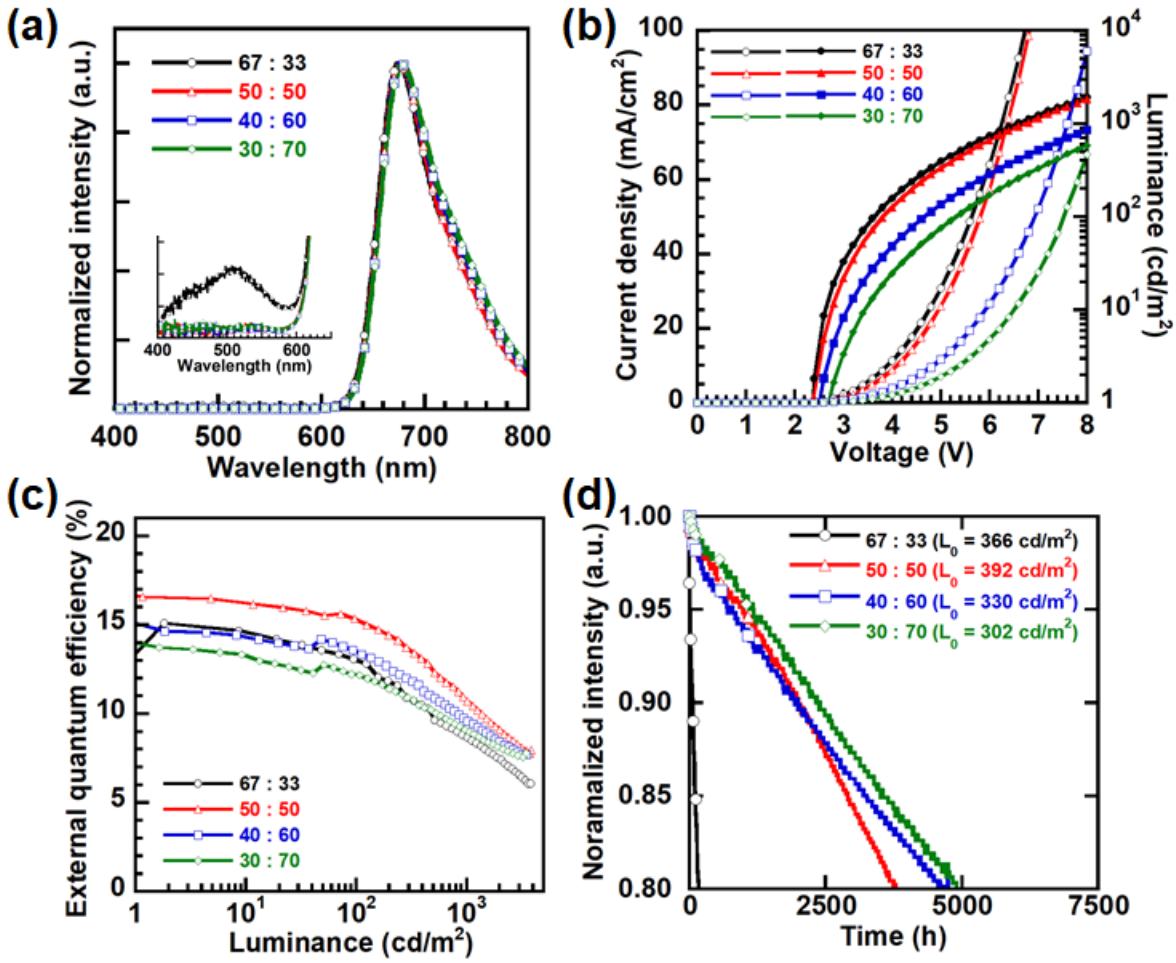

Figure S15 Device performances: (a) EL spectra at 1 mA (inset: EL spectra which enlarged short wavelength region), (b) J-V-L characteristics, (c) EQE-L characteristics and (d) Device lifetime under the constant current density of 25 mA cm^{-2}.

Table S1 Summery of OLED performances

	V_{on}/PE_{on}/CE_{on}/EQE_{on} [a] [V/lm W^{-1}/cd A^{-1}/%]	V_{100}/PE_{100}/CE_{100}/EQE_{100} [b] [V/lm W^{-1}/cd A^{-1}/%]	V_{1000}/PE_{1000}/ CE_{1000}/EQE_{1000} [c] [V/lm W^{-1}/cd A^{-1}/%]	*CIE* @ 25 mA/m^2	LT_{80} [d] [hs]
67 : 33	2.31/1.21/0.92/8.25	3.63/1.26/1.45/13.0	6.57/0.53/1.10/8.67	(0.61, 0.28)	172
50 : 50	2.37/2.16/1.63/16.7	3.82/1.20/1.46/15.3	6.73/0.49/1.06/10.8	(0.72, 0.28)	3800
40 : 60	2.47/1.81/1.42/15.3	4.66/0.81/1.20/13.5	8.33/0.33/0.88/9.65	(0.72, 0.28)	4700
30 : 70	2.67/1.53/1.30/14.1	5.31/0.63/1.06/12.2	9.09/0.28/0.80/9.06	(0.72, 0.28)	4920

[a] Voltage (*V*), power efficiency (PE), current efficiency (CE), and external quantum efficiency (EQE) at 1 $cdbm^{-2}$; [b] V, PE, CE, and EQE at 100 cd m^{-2}; [c] V, PE, CE and EQE at 1000 cd m^{-2}; [d] Operational lifetime: 20 % decay of initial luminance at current density of 25 mA/cm^2.