Supporting Information

Molecular Design of Thermally Activated Delayed Fluorescent

Emitters for Narrowband Orange-Red OLEDs: Boosted by a Cyano-

Functionalization Strategy

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Table of contents

I. General Remarks	3
II. OLED Fabrication and Characterization	3
III. Synthesis and Characterization	4
IV. Method of Theoretical Calculations	8
V. Crystal Data	9
VI. Additional Spectra and Data 1	10
VII. References 1	18
VIII. Copies of NMR spectra	22

I. General Remarks

All commercially available reagents and chemicals were used as received without further purification. Unless otherwise noted, all reactions were carried out using Schlenk techniques under a nitrogen atmosphere. The solvents were dried and purified using an Innovative Technology PS-MD-5 Solvent Purification System. NMR spectra were obtained on an Agilent 400-MR DD2 spectrometer. The ¹H NMR (400 MHz) chemical shifts were measured relative to CDCl₃ as the internal reference (CDCl₃: δ = 7.26 ppm). The ¹³C NMR (100 MHz) chemical shifts were given using CDCl₃ as the internal standard (CDCl₃: δ = 77.16 ppm). High-resolution mass spectra (HRMS) were obtained with a Shimadzu LCMS-IT-TOF (ESI). X-Ray single-crystal diffraction data were collected on an Oxford Xcalibur E single crystal diffraction. UV-Vis spectra were measured on a HITACHI U-2910. Fluorescence spectra and photoluminescence quantum yield were collected on a Horiba Jobin Yvon-Edison Fluoromax-3 spectrometer with a calibrated integrating fluorescence sphere system. Phosphorescence spectra were collected on a HITACHI F-7100 fluorescence spectrophotometer. Transient photoluminescence decay spectra were obtained with Horiba Single Photon Counting Controller: FluoroHub and Horiba TBX Picosecond Photon Detection. Thermogravimetric analysis (TGA) was carried out using DTG-60(H) at a rate of 10 °C/min under nitrogen atmosphere. Cyclic voltammogram were performed on LK2005A with a solution of tetrabutylammonium hexafluorophosphate (Bu₄NPF₆, 0.1 M) in DCM as electrolyte and ferrocene/ferrocenium (Fc/Fc⁺) as standard. Three-electrode system (Ag/Ag⁺, platinum wire and glassy carbon electrode as reference, counter and work electrode respectively) was used in the CV measurement.

II. OLED Fabrication and Characterization

Indium-tin-oxide (ITO) coated glass with a sheet resistance of 15 Ω sq⁻¹ was used as the anode substrate. Prior to film deposition, patterned ITO substrates were cleaned with alkaline detergent, boiled deionized water, and deionized water thoroughly in ultrasonic bath, dried in an oven, and finally treated with oxygen plasma for 10 min to enhance the surface work function of ITO anode. All of the organic layers were deposited with the rate of $0.1 \text{ nm} \cdot \text{s}^{-1}$ under high vacuum. The doped and co-doped layers were prepared by co-evaporating dopant and host material from two or three individual sources, and the doping concentrations were modulated by controlling the evaporation rates of dopant.

Measurements: Current density-voltage-Luminance (J-V-L) characteristics were measured by using KEYSIGHT B1500A. The luminance and EL spectra were collected with model DLM-100Z photometer and OPT2000 spectrophotometer, respectively.

III. Synthesis and Characterization



Scheme S1. Synthetic route to CNCz-BNCz. DMF: *N*,*N*-dimethylformamide; THF: tetrahydrofuran; EtN(*i*-Pr₂): *N*,*N*-diisopropylethylamine.

Synthesis of 9,9',9'',9'''-(3,6-Dibromobenzene-1,2,4,5-tetrayl)tetrakis(3,6-di-*tert*butyl-9*H*-carbazole) (compound 2). A dried round bottom flask with a magnetic stir bar was charged with 3,6-di-*tert*-butyl-9*H*-carbazole (6.29 g, 22.5 mmol), NaH (1.08 g, 60%, 27.0 mmol), and 50 mL of DMF under an air atmosphere. After stirring for 0.5 h under room temperature, 1,4-dibromotetrafluorobenzene (1.54 g, 5 mmol) was added to the reaction mixture and stirred for 12 h at 140 °C. After cooling to room temperature, the mixture was filtered and the solid was washed with DMF. The residue was dissolved in THF and the insoluble matter was filtered off. The product was evaporated under reduced pressure to provide compound 2 as a white solid in 95% yield (6.39 g, 4.75 mmol). ¹H NMR (CDCl₃, 400 MHz): $\delta = 1.38$ (s, 72H), 6.97 (d, J = 8.4 Hz, 8H), 7.09 (dd, $J_1 = 8.4$ Hz, $J_2 = 2.0$ Hz, 8H), 7.61 (d, J = 2.0 Hz, 8H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 32.1$, 34.7, 110.2, 115.6, 122.7, 123.9, 129.6, 137.2, 138.5, 143.1 ppm. HRMS (ESI⁺): calcd for C₈₆H₉₆Br₂N₄Na [M+Na]⁺, 1367.5879 (100%), 1368.5913 (79.0%), 1365.5899 (51.4%), 1369.5859 (48.6%); found 1367.5875, 1368.5910, 1365.5874, 1369.5885.

Synthesis of BrCz-BNCz (compound 3). In a dried round bottom flask with a magnetic stir bar, a solution of *n*-BuLi in hexane (1.05 mL, 2.5 M, 2.625 mmol) was added slowly to a solution of compound 2 (3.36 g, 2.5 mmol) in toluene (100 mL) at -60 °C under a nitrogen atmosphere. After stirring for 1.0 h the reaction mixture was allowed to warm to -40 °C. After addition of boron tribromide (0.355 mL, 3.75 mmol), the reaction mixture was stirred at room temperature for 1.0 h. N,N-Diisopropylethylamine (1.75 mL, 10.0 mmol) was added at 0 °C and then the reaction mixture was allowed to warm to 120 °C. After stirring for 8 h, the reaction mixture was cooled to room temperature. The solution was filtered through a celite pad and washed with dichloromethane. The filtrate was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 20:1, v/v) and recrystallized from dichloromethane and methanol as orange powder in 45% yield (1.43 g, 1.125 mmol). ¹H NMR (400 MHz, CDCl₃): $\delta = 1.21$ (s, 18H), 1.42 (s, 36H), 1.70 (s, 18H), 6.14 (dd, $J_1 = 8.8$ Hz, $J_2 = 2.0$ Hz, 2H), 6.63 (d, J = 8.8 Hz, 2H), 7.17 (br, 8H), 7.55 (d, J = 2.0Hz, 2H), 7.85 (s, 4H), 8.26 (d, J = 1.6 Hz, 2H), 9.17 (d, J = 2.0 Hz, 2H) ppm. ¹³C NMR $(100 \text{ MHz}, \text{CDCl}_3)$: $\delta = 31.6, 32.1, 32.3, 34.4, 34.8, 35.4, 113.4, 114.8, 116.0, 120.4, 110.0, 120.4, 12$ 121.6, 121.7, 122.2, 123.5, 125.1, 125.2, 129.0, 129.5, 136.8, 137.5, 137.6, 141.7, 142.9, 143.3, 145.0, 145.4 ppm. HRMS (ESI⁺): calcd for C₈₆H₉₅BBrN₄ [M+H]⁺, 1273.6833 (100.0%), 1275.6813 (97.3%); found 1273.6844, 1275.6814.

Synthesis of CNCz-BNCz (compound 4).^[1] In a dried round bottom flask with a magnetic stir bar, a solution of *n*-BuLi in hexane (0.44 mL, 2.5 M, 1.1 mmol) was added slowly to a solution of compound **3** (1.274 g, 1.0 mmol) in THF (30 mL) at -78 °C under a nitrogen atmosphere. After stirring for 1.0 h, dimethylmalononitrile

(141.2 mg, 1.5 mmol) was added and then the reaction mixture was allowed to slowly warm to room temperature. After stirring for 8 h at room temperature, the solution was filtered through a celite pad and washed with dichloromethane. The filtrate was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 5:1, v/v) and recrystallized from dichloromethane and methanol as red powder in 26% yield (317.4 mg, 0.26 mmol). ¹H NMR (400 MHz, CDCl₃): δ = 1.20 (s, 18H), 1.41 (s, 36H), 1.71 (s, 18H), 6.19 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 2H), 6.56 (d, J = 8.8 Hz, 2H), 7.00 (br, 4H), 7.32 (br, 4H), 7.59 (d, J = 1.6 Hz, 2H), 7.87 (s, 4H), 8.31 (d, J = 1.6Hz, 2H), 9.19 (d, J = 1.6Hz, 2H) ppm. ¹³C NMR (100 MHz, CDCl₃): δ = 31.6, 32.1, 32.3, 34.4, 34.8, 35.5, 108.7, 113.0, 114.7, 115.1, 116.4, 120.5, 122.1, 122.2, 122.7, 123.7, 123.9, 124.6, 125.2, 125.3, 129.3, 136.8, 137.8, 139.9, 143.1, 143.5, 145.5, 146.0 ppm. HRMS (ESI⁺): calcd for C₈₇H₉₅BN₅ [M+H]⁺1220.7681, found 1220.7678. Anal. Calcd (%) C₈₇H₉₄BN₅: C, 85.61; H, 7.76; N, 5.74; Found: C, 85.59; H, 7.73; N, 5.83. (B is not analyzed by elemental analysis)



Scheme S2. Synthetic route to **CN-BCz-BN**. DMF: *N*,*N*-dimethylformamide; THF: tetrahydrofuran.

Synthesis of 9,9'-(5-Bromo-2-iodo-1,3-phenylene)bis(3,6-di-*tert***-butyl-9***H***-carbazole) (compound 5).** A dried round bottom flask with a magnetic stir bar was charged with 3,6-di-*tert*-butyl-9*H*-carbazole (3.35 g, 12 mmol), NaH (576 mg, 60%, 14.4 mmol), and DMF 50 mL under an air atmosphere. After stirring for 0.5 h under room temperature, 4-bromo-2,6-difluoroiodobenzene (1.56 g, 5 mmol) was added to

the reaction mixture and stirred for 12 h at 140 °C. After cooling to room temperature, the solution was filtered through a celite pad and washed with dichloromethane. The filtrate was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 10:1, v/v) to provide compound **5** as a white solid in 78% yield (3.27 g, 3.9 mmol). ¹H NMR (CDCl₃, 400 MHz): $\delta = 1.49$ (s, 36H), 7.12 (d, J = 8.8 Hz, 4H), 7.53 (dd, $J_I = 8.4$ Hz, $J_2 = 2.0$ Hz, 4H), 7.69 (s, 2H), 8.17 (d, J = 2.0 Hz, 4H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 32.2$, 35.0, 104.3, 109.6, 116.7, 123.4, 123.6, 124.1, 133.5, 139.0, 143.5, 144.7 ppm. HRMS (ESI⁺): calcd for C₄₆H₅₀BrIN₂Na [M+Na]⁺, 859.2100 (100.0%), 861.2079 (97.3%); found 859.2085, 861.2080.

Synthesis of Br-BCz-BN (compound 6). In a dried round bottom flask with a magnetic stir bar, a solution of *n*-BuLi in hexane (1.05 mL, 2.5 M, 2.625 mmol) was added slowly to a solution of 9,9'-(5-bromo-2-iodo-1,3-phenylene)bis(3,6-di-tert-butyl-9Hcarbazole) (compound 5) (2.1 g, 2.5 mmol) in toluene (50 mL) at -60 °C under a nitrogen atmosphere. After stirring for 1.0 h the reaction mixture was allowed to warm to -40 °C. After addition of boron tribromide (0.355 mL, 3.75 mmol), the reaction mixture was stirred at room temperature for 1.0 h. N, N-Diisopropylethylamine (1.75 mL, 10.0 mmol) was added at 0 °C and then the reaction mixture was allowed to warm to 120 °C. After stirring for 8 h, the reaction mixture was cooled to room temperature. The solution was filtered through a celite pad and washed with dichloromethane. The filtrate was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 5:1, v/v) to provide compound 6 as yellow powder in 42% yield (755 mg, 1.05 mmol). ¹H NMR (400 MHz, CDCl₃): δ = 1.53 (s, 18H), 1.67 (s, 18H), 7.60 (dd, $J_1 = 8.8$ Hz, $J_2 = 2.0$ Hz, 2H), 8.13 (dd, $J_1 = 8.8$ Hz, $J_2 =$ 1.6 Hz, 2H), 8.16 (d, J = 2.0 Hz, 2H), 8.20 (d, J = 1.6 Hz, 2H), 8.38 (d, J = 1.6 Hz, 2H), 9.00 (d, J = 2.0 Hz, 2H) ppm. ¹³C NMR (100 MHz, CDCl₃): $\delta = 32.0, 32.3, 34.9, 35.3,$ 110.8, 114.1, 117.3, 120.9, 121.5, 123.7, 124.6, 127.2, 127.7, 129.8, 138.0, 141.4, 144.6, 144.9, 145.6 ppm. HRMS (ESI⁺): calcd for C₄₆H₄₉BBrN₂ [M+H]⁺, 719.3172 (100.0%),

721.3152 (97.3%); found 719.3169, 721.3153.

Synthesis of CN-BCz-BN (compound 7). A dried round bottle flask with a magnetic stir bar was charged with compound 6 (144 mg, 0.2 mmol), and CuCN (26.9 mg, 0.3 mmol) in DMF (5 mL) at 150 °C under nitrogen atmosphere for 12 h. After cooling to room temperature, the solution was filtered through a celite pad and washed with dichloromethane. The filtrate was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel (petroleum ether/dichloromethane = 2:1, v/v) to provide compound 7 as a yellow solid in 58% yield (77.2 mg, 0.116 mmol). ¹H NMR (400 MHz, CDCl₃): δ = 1.54 (s, 18H), 1.67 (s, 18H), 7.65 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 2H), 8.20-8.22 (m, 4H), 8.34 (s, 2H), 8.44 (d, J = 2.0 Hz, 2H), 9.03 (d, J = 2.0 Hz, 2H) ppm. ¹³C NMR (100 MHz, CS₂/CDCl₃ = 1:1, v/v): δ = 31.8. 32.1, 34.6, 35.0, 110.2, 114.0, 115.9, 117.6, 119.1, 121.5, 124.0, 124.9, 127.2, 129.9, 137.8, 141.2, 144.0, 145.2, 146.0 ppm. HRMS (ESI⁺): calcd for C₄₇H₄₉BN₃ [M+H]⁺ 666.4020, found 666.4018. Anal. Calcd (%) C₄₇H₄₈BN₃: C, 84.80; H, 7.27; N, 6.31; Found: C, 84.57; H, 7.17; N, 6.29. (B is not analyzed by elemental analysis)

IV. Method of Theoretical Calculations

All theoretical calculations were performed using Gaussian $09^{[2]}$ serials software. The ground-state structures and FMOs were obtained by B3LYP^[3] density functional method with basis set 6-31G*. The S₁ and T₁ energies were calculated by timedependent DFT (TD-DFT) method with the same parameters for ground-state calculations. The HOMO and LUMO distributions were visualized using Gaussview 5.0 software.

V. Crystal Data

Table S.	1. Crystal	Data for	CNCz-BNCz

Identification code	CNCz-BNCz
Empirical formula	C ₈₇ H ₉₄ BN ₅
Formula weight	1220.48
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	18.299(3)
b/Å	29.627(5)
c/Å	14.364(3)
α/°	90
β/°	104.263(10)
$\gamma/^{\circ}$	90
Volume/Å ³	7547(2)
Ζ	4
$\rho_{calc}g/cm^3$	1.074
μ/mm^{-1}	0.466
F(000)	2624.0
Crystal size/mm ³	0.3 imes 0.2 imes 0.2
Radiation	$CuK\alpha$ ($\lambda = 1.54178$)
2Θ range for data collection/°	4.982 to 138.382
Index ranges	$-21 \le h \le 22, -35 \le k \le 33, -17 \le l \le 17$
Reflections collected	75860
Independent reflections	13757 [$R_{int} = 0.0992, R_{sigma} = 0.0888$]
Data/restraints/parameters	13757/0/929
Goodness-of-fit on F ²	1.068
Final R indexes [I>= 2σ (I)]	$R_1 = 0.0923, wR_2 = 0.2561$
Final R indexes [all data]	$R_1 = 0.1416, wR_2 = 0.3044$
Largest diff. peak/hole / e Å ⁻³	0.50/-0.33



VI. Additional Spectra and Data

Fig. S1. Theoretical calculation results of the FMOs distributions and energy levels of BCz-BN, CN-BCz-BN, *m*-Cz-BBCz, BBCz-Y and CNCz-BNCz.



Fig. S2. Emissions of BCz-BN, CN-BCz-BN, BBCz-Y and CNCz-BNCz in toluene solution at 1×10^{-5} mol L⁻¹.



Fig. S3. (a) TGA thermogram of CNCz-BNCz recorded at a heating rate of 10 °C/min.
(b) Cyclic voltammograms of CNCz-BNCz, measured in dry dichloromethane containing 0.1 M of tetrabutylammonium hexafluorophosphate.



Fig. S4. (a) Normalized UV-vis absorption spectrum of CNCz-BNCz and (b) normalized photoluminescence spectrum of CNCz-BNCz in solvents with different polarity at 2×10^{-5} mol L⁻¹.



Fig. S5. (a) Normalized UV-vis absorption spectrum of CNCz-BNCz and (b) normalized photoluminescence spectrum of CNCz-BNCz in toluene solution at different concentrations.



Fig. S6. Normalized photoluminescence spectrum of **CNCz-BNCz** in in PS at different concentrations.



Fig. S7. (a) Fluorescence spectrum and (b) phosphorescence spectrum of **CNCz-BNCz** in PS (3 wt% doped film) at different temperature.



Fig. S8. Fluorescence spectrum of CNCz-BNCz in polystyrene film (3 wt%) at room temperature (298 K) and 77 K.



Fig. S9. (a) Fluorescence spectrum and (b) transient photoluminescence spectrum of CNCz-BNCz in CBP film (3 wt%) at 298 K.



Fig. S10. Current density and luminance versus voltage curves of Device A, B and C.



Fig. S11. (a) EL spectra at the luminance of 1000 cd m⁻². (b) EQE and power efficiency versus luminance curves of doped OLEDs and (c) Current density and luminance versus voltage curves. Devices configuration: ITO/TAPC (30 nm)/TCTA (10 nm)/32alCTRZ: 20 wt% DACT-II: *x* wt% **CNCz-BNCz** (20 nm)/TmPyPb (50 nm)/LiF (0.8 nm)/Al, where *x* is 1, 2, 3 and 5 for device D, E, C and F, respectively.



Fig. S12. Histogram of EQEs_{max}. An average EQE_{max} of 29.2% and a highest EQE_{max} of 33.7%.

Compound	$T_{\rm d}$	HOMO ^[a]	LUMO ^[b]	$\lambda_{abs}^{[c]}$	$\lambda_{\rm em}^{[c]}$
	[°C]	[eV]	[eV]	[nm]	[nm]
CNCz-BNCz	409	-5.33	-3.19	345/547	581
Compound	$E_{ m g}{}^{[d]}$	$E_{S1}^{[e]}$	$E_{\mathrm{T1}}^{\mathrm{[f]}}$	$\Delta E_{\rm ST}^{[g]}$	$arPsi_{ ext{PL}}{}^{[ext{h}]}$
	[eV]	[eV]	[eV]	[eV]	[%]
CNCz-BNCz	2.14	2.28	2.10	0.18	90

Table S2: Summary of physical properties for CNCz-BNCz.

[a] Measured in dry dichloromethane solution $(1 \times 10^{-3} \text{ M})$ where $E_{\text{HOMO}} = -4.8 - (E_{\text{ox}} - E_{\text{Fc}})$. [b] Estimated according to the absorption spectrum and the HOMO energy level. [c] Measured in toluene solution $(1 \times 10^{-5} \text{ M})$ at room temperature. [d] Calculated from the absorption spectrum. [e] Estimated from the onset wavelength of room-temperature photoluminescence measured in toluene solution $(1 \times 10^{-5} \text{ M})$. [f] Estimated from the onset wavelength of low-temperature photoluminescence measured in toluene solution $(1 \times 10^{-5} \text{ M})$. [f] Estimated from the onset wavelength of $1 \times 10^{-5} \text{ M}$ at 77 K. [g] Calculated from E_{S1} and E_{T1} . [h] Measured in oxygen-free toluene solution $(1 \times 10^{-5} \text{ M})$.

Table S3: Transient PL decay data of CNCz-BNCz in toluene solution $(1 \times 10^{-5} \text{ M})$ measured at room temperature under nitrogen atmosphere.

Compound	$\tau_{p}^{[a]}$	τ _d ^[b]	C ₁ ^[c]	C ₂ ^[d]	$k_{\rm RISC}^{[e]}$	$k_{\rm r}^{\rm [f]}$	$k_{\rm ISC}^{\rm [g]}$
	[ns]	[μs]	[%]	[%]	[×10 ⁵ s ⁻¹]	[×10 ⁷ s ⁻¹]	[×10 ⁷ s ⁻¹]
CNCz-BNCz	28.4	3.4	70.2	29.8	4.2	2.2	1.1

[a] Prompt lifetime. [b] Delayed lifetime. The proportion of [c] prompt and [d] delayed components which are calculated from transient spectra. [e] Calculated from $k_{\text{RISC}} = 1/(C_1 \tau_d)$. [f] Calculated from $k_r = C_1 \Phi_{\text{PL,N2}}/\tau_p$. [g] Calculated from $k_{\text{ISC}} = (1-C_1)/\tau_p$.

Table S4: Summary of photophysical properties for CNCz-BNCz in CBP film (3 wt%).

Compound	λ _{em} [nm]	$\Phi_{ m PL}$ [%]	$\tau_{\rm p}$	$\tau_{\rm d}$ [us]
CNCz-BNCz	582	96	17.7	60.4

			DE [c]		at 10	0 cd m ⁻²	at 10	at 1000 cd m ⁻²		
Device	EL _{peak} [nm]	[V]	rwnw [nm]	[%]	[lm W ⁻¹]	[x, y]	EQE [%]	PE [lm W ⁻¹]	EQE [%]	PE [lm W ⁻¹]
С	583	2.7	49	33.7	117.8	[0.54, 0.46]	27.7	69.1	16.4	29.6
D	577	2.6	49	27.9	107.5	[0.50, 0.49]	21.3	61.8	14.2	32.1
Е	581	2.7	50	27.7	94.8	[0.53, 0.47]	22.6	57.8	13.5	25.6
F	584	2.7	51	27.8	83.0	[0.55, 0.45]	21.2	51.8	9.8	16.5

Table S5: Summary of EL characteristics for OLED devices.

[a] Turn-on voltage. [b] External quantum efficiency. [c] Power efficiency. [d] Commission Internationale de l'Eclairage (CIE) coordinates. Current density and luminance versus voltage curves. Devices configuration: ITO/TAPC (30 nm)/TCTA (10 nm)/32alCTRZ: 20 wt% DACT-II: x wt% **CNCz-BNCz** (20 nm)/TmPyPb (50 nm)/LiF (0.8 nm)/Al., where x is 1, 2, 3 and 5 for device D, E, C and F, respectively.

Table S6: Performance summary of TADF-OLEDs with emission peaks from 550 nm to 650 nm.

F	EL _{peak} [a]	FWHM	$V_{on}^{[b]}$	CE _{max} ^[c]	PE _{max^[d]}	EQE _{max} ^[e]	$EQE_{100}^{\left[f\right]}$	Dí
Emitter	[nm]	[nm]	[V]	[cd A ⁻¹]	[lm W ⁻¹]	(%)	(%)	Reference
CNCz-BNCz	583	49	2.7	101.3	117.8	33.7	27.7	This work
QBP-PXZ	550		3.4	53.6	52.6	16.6	15.2	4
FDQCNAc	554			90.8	91.6	27.6		5
SBPQ-DPAC	556		3.2	65.7	59.0	20.0	19.0	6
25DAcBPy	558		3.5	71.6	59.7	19.6		7
Me-PXZ	562		3.0	54.4	48.2	21.1		8
SpAcDBA	567	96	3.0	84.7	76.6	29.5	28.9	9
6,7-DCNQx-DICz	578			63.1	62.3	23.9		10
6,7-DCQx-Ac	578			56.8	50.9	21.1		11
Ac-CNP	580		4.7	38.1	26.1	13.3	12.0	12
3,6,11-TriAC-BPQ	581		2.9	44.2	46.3	22.0		13
dmAcDBA	583	98	3.2	58.3	48.6	24.9	23.1	9
NAI-DPAC	584		3.0	76.2	79.7	29.2	13.0	14
Ac-CNBQx	585		2.8	34.0	33.3	14.0	13.9	15
DMAC-11-DPPZ	588	95	3.6	50.8	41.0	23.8		16
NP	590	114	3.6	28.6	23.2	17.1		17
BFDMAc-NAI	590		3.0	49.2	51.4	20.3	10.6	18
1PXZ-BP	590	106	2.6	47.2	57.1	26.3	17.2	19
DPXZ-PQM	590		2.8	60.7	67.4	26.0	20.1	20
T-DA-1	596		3.0	51.2	53.6	22.6	14.1	21
DMAC-Ph-DCPP	596		3.3	34.5	32.8	16.9		22
NAI-DMAC	597		3.0	50.7	53.1	23.4	13.6	14
FBPCNAc	597			55.7	57.8	23.8		5
oTPA-DPPZ	600		3.1	41.8	42.3	18.5	17.0	23
BPPZ-PXZ	604			37.0	41.0	25.2	21.0	24
oDTBPZ-DPXZ	604		3.5	38.1	29.2	20.1	14.1	25
3DMAC-BP	606	90	3.1	38.2	36.4	22.0	17.5	26
W1	608		4.1	40.0	38.3	25.0	8.7	27
HAP-3TPA	609			25.9	22.1	17.5	12.8	28
POZ-DBPHZ	610					16.0		29
DPXZ-BPPZ	612		3.1	30.2	30.9	20.1	19.6	30
ANQDC-DMAC	615		2.7	47.6	53.1	27.5	19.3	31
NAI_R3	622		7.0	28.3	9.4	22.5		32
mDPBPZ-PXZ	624			25.0	21.0	21.7	19.0	24
B1	624					12.5	8.1	33
TPAAQ	630					15.8	2.8	34
B2	637					9.0	5.7	33
				S17				

T-DA-2	640	 3.0	24.4	22.5	26.3	24.0	21
TPA-QCN	644	 3.0	14.3	14.9	14.5		35
TPA-PZCN	648	 2.4	20.0	26.3	28.1	6.4	36

[a] Emission peak. [b] Turn-on voltage. [c] Maximum current efficiency. [d] Maximum Power efficiency. [e] Maximum External quantum efficiency. [f] External quantum efficiency at 100 cd m⁻².

VII. References

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VIII. Copies of NMR spectra

¹H NMR spectra of **2** (CDCl₃)



¹³C NMR spectra of **2** (CDCl₃)



¹H NMR spectra of **3** (CDCl₃)





¹³C NMR spectra of **3** (CDCl₃)



110 100 f1 (ppm) 210 200 190 180 170 160 150 140 130 120 -1

¹H NMR spectra of 4 (CDCl₃)



¹³C NMR spectra of 4 (CDCl₃)



¹H NMR spectra of **5** (CDCl₃)



¹³C NMR spectra of **5** (CDCl₃)



¹H NMR spectra of **6** (CDCl₃)



¹³C NMR spectra of **6** (CDCl₃)



¹H NMR spectra of 7 (CDCl₃)



¹³C NMR spectra of 7 (CDCl₃)

