

Electronic Supplementary Information (ESI)

## **Molecular engineering of phosphacycle-based thermally activated delayed fluorescence materials for deep-blue OLEDs**

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**Materials and methods.** Commercially available reagents and solvents were used as received unless otherwise noted. Spiro[2,7-dimethylacridan-9-9'-fluorene] (MFAc),<sup>1</sup> 1,4-dibromo-2-(2-bromophenoxy)benzene (**6b**),<sup>2</sup> 9-phenyl-3,9'-bicarbazole (CCP),<sup>2</sup> and 2,8-bis(diphenylphosphoryl)dibenzo[*b,d*]furan (PPF)<sup>3</sup> were prepared according to the literature procedures. 2,3,6,7,10,11-Hexacyano-1,4,5,8,9,12-hexaazatriphenylene (HAT-CN) was donated by the Nippon Soda Co., Ltd. and was purified using vacuum sublimation before use. Other OLED materials were purchased from e-Ray Optoelectronics Technology Co., Ltd., and were used for the device fabrication without further purification.

NMR spectra were recorded on an Avance III 500 and 400 spectrometers (Bruker). Chemical shifts of NMR signals were referenced to tetramethylsilane ( $\delta = 0.00$ ),  $\text{CDCl}_3$  ( $\delta = 77.0$ ), and  $\text{DMSO-}d_6$  ( $\delta = 39.5$ ), as internal standards. Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectra were collected on an Autoflex III spectrometer (Bruker Daltonics) using dithranol as a matrix. Elemental analyses were performed using an MT-5 analyzer (Yanaco).

**Quantum chemical calculations.** Density functional theory (DFT) calculations were performed using the Gaussian 09 program package. The molecular geometries in the ground state were optimized using the PBE0 functional with the 6-31G(d) basis set in the gas phase. The lowest singlet and triplet excited states were computed using the optimized structures with time-dependent DFT (TDDFT) at the same level.

**Photophysical characterizations.** Organic thin films for photophysical measurements were prepared by vacuum deposition under high vacuum ( $\sim 7 \times 10^{-5}$  Pa) onto a quartz glass or Si(100) substrate. UV-vis absorption and photoluminescence (PL) spectra were measured using a V-670 spectrometer (Jasco) and a FP-8600 spectrophotometer (Jasco), respectively, using degassed spectral grade solvents. The absolute PL quantum yields ( $\Phi_{\text{PL}}$ ) were determined using an ILF-835 integrating sphere system (Jasco). The transient PL characteristics were performed using a C11367 Quantaaurus-Tau fluorescence lifetime spectrometer (Hamamatsu Photonics;  $\lambda_{\text{ex}} = 340$  nm, pulse width = 100 ps, and repetition rate = 20 Hz) under  $\text{N}_2$  atmosphere. The HOMO energy levels of materials in the thin films were determined using an AC-2 ultraviolet photoelectron spectrometer (Riken-Keiki). The LUMO energy levels were estimated by subtracting the optical energy gap ( $E_{\text{g}}$ ) from the measured HOMO energy levels; the  $E_{\text{g}}$  values were determined from the high energy onset position of the PL spectra of the thin films.

**OLED fabrication and measurements.** Indium tin oxide (ITO)-coated glass substrates were cleaned with detergent, deionized water, acetone, and isopropyl alcohol, and then subjected to UV-ozone treatment for 30 min, before loading into an E-200 vacuum evaporation system (ALS technology). The organic layers and a cathode aluminum layer were thermally evaporated on the substrates under vacuum ( $< 6 \times 10^{-5}$  Pa) with an evaporation rate of  $< 0.3 \text{ nm s}^{-1}$  through a shadow mask. The layer thickness and deposition rates were monitored *in situ* during deposition by an oscillating quartz thickness monitor. OLED characteristics were measured using a Keithley 2400 source meter and a CS-2000 spectroradiometer (Konica Minolta).

**Synthesis of 6a:** To a stirred mixture of 2-bromothiophenol (9.5 g, 50.2 mmol) and  $\text{K}_2\text{CO}_3$  (13.8 g, 99.8 mmol) in triethylene glycol dimethyl ether (10 mL) was added 1,4-dibromo-2-fluorobenzene (15.2 g, 59.9 mmol). The mixture was stirred at 180 °C for 24 h under  $\text{N}_2$ . After cooling to room temperature, toluene (100 mL) was added to the reaction mixture, and then the reaction mixture was extracted with toluene. The combined organic layers were washed with water, and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . After filtration and evaporation, the product was purified by column chromatography on silica gel (eluent:  $\text{CHCl}_3/\text{hexane} = 1/3$ , v/v) and dried under vacuum to afford a white solid (yield = 14.0 g, 66%).  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.70 (dd,  $J = 8.0 \text{ Hz}$ ,  $0.8 \text{ Hz}$ , 1H), 7.46 (d,  $J = 8.4 \text{ Hz}$ , 1H), 7.34–7.29 (m, 2H), 7.25–7.20 (m, 2H), 7.06 (d,  $J = 2.0 \text{ Hz}$ , 1H). MS (MALDI-TOF):  $m/z$  calcd 419.78 [ $M$ ] $^+$ ; found 419.96.

**Synthesis of MFAc-SPO (2).** To a stirred solution of **6a** (8.07 g, 19.1 mmol) in dry diethyl ether (450 mL) was added dropwise *n*-butyllithium (1.6 M, 26.3 mL, 42.0 mmol) at  $-78 \text{ }^\circ\text{C}$ . The mixture was allowed to react for 1 h at  $-78 \text{ }^\circ\text{C}$ . Dichlorophenylphosphine (3.76 g, 21.0 mmol) was then added, and the mixture was stirred overnight at room temperature. Hydrogen peroxide (ca. 30%, 1.5 mL) was added dropwise in to the solution, and the mixture was stirred for 2 h at room temperature. The reaction mixture was then poured into water and extracted with ethyl acetate. The combined organic layers were washed with water, and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The solution was filtered through a Celite pad, and the filtrate was concentrated by evaporation. The crude product of **5a** was used in the next reaction.

To a stirred solution of **5a** (4.65 g, 12.0 mmol) and spiro[2,7-dimethylacridan-9,9'-fluorene] (4.32 g, 12.0 mmol) in dry toluene (150 mL) were added palladium(II) acetate

(Pd(OAc)<sub>2</sub>; 0.08 g, 0.36 mmol), tri-*tert*-butylphosphonium tetrafluoroborate (P(*t*-Bu)<sub>3</sub>HBF<sub>4</sub>; 0.52 g, 1.79 mmol), and sodium *tert*-butoxide (*t*-BuONa; 2.77 g, 28.8 mmol). The mixture was refluxed for 24 h under N<sub>2</sub>. After cooling to room temperature, the reaction mixture was poured into water and then extracted with CHCl<sub>3</sub>. The combined organic layers were washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After filtration and evaporation, the product was purified by silica-gel column chromatography (eluent: CH<sub>2</sub>Cl<sub>2</sub>), recrystallized from CH<sub>2</sub>Cl<sub>2</sub>/hexane, and dried under vacuum to afford MFAc-SPO as a light yellow solid (3.94 g, 31%). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.46 (d, *J* = 8.4 Hz, 0.5H), 8.43 (d, *J* = 8.4 Hz, 0.5H), 8.17 (dd, *J* = 7.2 Hz, 1.6 Hz, 0.5H), 8.14 (dd, *J* = 7.2 Hz, 1.6 Hz, 0.5H), 8.02 (dd, *J* = 8.4 Hz, 2.0 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 2H), 7.81–7.78 (m, 2H), 7.74–7.66 (m, 2H), 7.62–7.57 (m, 1H), 7.55–7.46 (m, 4H), 7.42 (td, *J* = 7.2 Hz, 1.2 Hz, 2H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.30 (td, *J* = 7.6 Hz, 1.2 Hz, 2H), 6.77 (dd, *J* = 8.8 Hz, 2.0 Hz, 2H), 6.20 (d, *J* = 8.8 Hz, 2H), 6.02 (d, *J* = 2.0 Hz, 2H), 1.87 (s, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 157.69 (d, *J*<sub>CP</sub> = 3.6 Hz), 156.23, 155.74 (d, *J*<sub>CP</sub> = 3.0 Hz), 147.01, 139.30, 138.60, 134.13, 134.01 (d, *J*<sub>CP</sub> = 5.3 Hz), 133.10, 132.13, 131.85 (d, *J*<sub>CP</sub> = 10.8 Hz), 131.47 (d, *J*<sub>CP</sub> = 5.3 Hz), 130.11, 128.75 (d, *J*<sub>CP</sub> = 13.0 Hz), 128.39, 128.04 (d, *J*<sub>CP</sub> = 3.5 Hz), 127.56, 127.20 (d, *J*<sub>CP</sub> = 10.6 Hz), 125.75, 124.95, 124.54 (d, *J*<sub>CP</sub> = 10.4 Hz), 121.24 (d, *J*<sub>CP</sub> = 6.3 Hz), 119.90, 118.46 (d, *J*<sub>CP</sub> = 5.9 Hz), 115.89 (d, *J*<sub>CP</sub> = 31.1 Hz), 115.08 (d, *J*<sub>CP</sub> = 32.6 Hz), 114.46, 56.81, 20.40. MS (MALDI-TOF): *m/z* calcd 665.19 [*M*]<sup>+</sup>; found 665.24. Anal. calcd (%) for C<sub>38</sub>H<sub>25</sub>NO<sub>2</sub>: C 81.18, H 4.84, N 2.10; found: C 81.00, H 4.81, N 2.16.

**Synthesis of MFAc-SPS (1).** A mixture of MFAc-SPO (2.50 g, 3.75 mmol) and Lawesson's reagent (3.04 g, 7.52 mmol) in dry toluene (150 mL) was refluxed for 24 h under N<sub>2</sub>. After cooling the room temperature, the solvent was removed under reduced pressure. The crude product was purified by column chromatography on silica gel (hexane/CHCl<sub>3</sub> = 1/1, v/v), and recrystallized from CH<sub>2</sub>Cl<sub>2</sub>/hexane, and dried under vacuum to afford MFAc-SPS as a light yellow solid (yield = 1.76 g, 69%). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.75 (d, *J* = 8.4 Hz, 0.5H), 8.72 (d, *J* = 8.4 Hz, 0.5H), 8.48 (dd, *J* = 7.2 Hz, 1.6 Hz, 0.5H), 8.44 (dd, *J* = 7.2 Hz, 1.6 Hz, 0.5H), 8.04 (dd, *J* = 8.4 Hz, 1.6 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 2H), 7.85 (dt, *J* = 8.4 Hz, 1.6 Hz, 1H), 7.83–7.72 (m, 3H), 7.55–7.50 (m, 1H), 7.48–7.41 (m, 4H), 7.38 (d, *J* = 7.2 Hz, 2H), 7.35–7.28 (m, 4H), 6.78 (dd, *J* = 8.4 Hz, 2.0 Hz, 2H), 6.22 (d, *J* = 8.4 Hz, 2H), 6.03 (d, *J* = 2.0 Hz, 2H), 1.88 (s, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 156.21, 144.82 (d, *J*<sub>CP</sub> = 3.0 Hz), 140.16 (d, *J*<sub>CP</sub> = 6.3 Hz), 139.28, 138.64, 137.14 (d, *J*<sub>CP</sub> = 5.4 Hz), 136.65 (d, *J*<sub>CP</sub> = 11.3 Hz), 134.16 (d, *J*<sub>CP</sub>

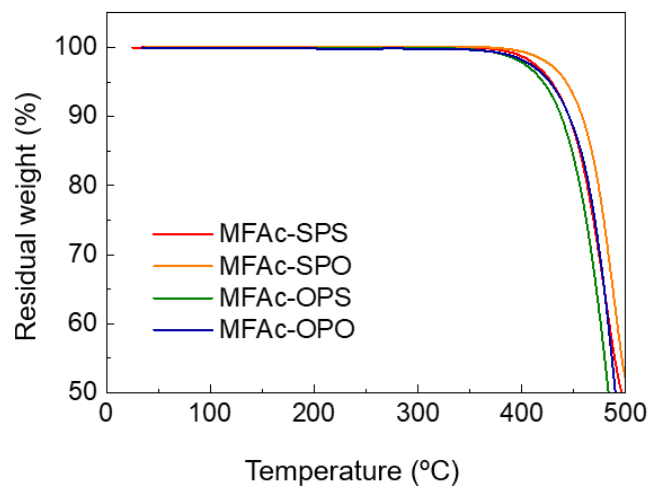
= 10.8 Hz), 133.16, 132.45, 131.71 (d,  $J_{CP}$  = 2.1 Hz), 131.47 (d,  $J_{CP}$  = 2.9 Hz), 130.63 (d,  $J_{CP}$  = 12.3 Hz), 130.60 (d,  $J_{CP}$  = 11.3 Hz), 130.47 (d,  $J_{CP}$  = 7.6 Hz), 130.14, 128.67 (d,  $J_{CP}$  = 13.2 Hz), 128.39, 128.06, 127.87 (d,  $J_{CP}$  = 6.4 Hz), 127.79, 127.57, 127.53 (d,  $J_{CP}$  = 43.1 Hz), 126.84 (d,  $J_{CP}$  = 43.8 Hz), 125.72, 124.97, 119.90, 114.38, 56.78, 20.39. MS (MALDI-TOF):  $m/z$  calcd 681.17 [ $M$ ]<sup>+</sup>; found, 681.27. Anal. calcd (%) for C<sub>38</sub>H<sub>25</sub>NO<sub>2</sub>: C 79.27, H 4.73, N 2.05; found: C 79.28, H 4.70, N 2.11.

**Synthesis of MFAc-OPO (4).** To a stirred solution of 1,4-dibromo-2-(2-bromophenoxy)benzene (6.85 g, 16.8 mmol) in dry diethyl ether (300 mL) was added dropwise *n*-butyllithium (1.6 M, 23.1 mL, 37.0 mmol) at -78 °C. The mixture was allowed to react for 1 h at -78 °C. Dichlorophenylphosphine (3.31 g, 18.5 mmol) was then added, and the mixture was stirred overnight at room temperature. Hydrogen peroxide (ca. 30%, 1.0 mL) was added dropwise in to the solution, and the mixture was stirred for 2 h at room temperature. The reaction mixture was then poured into water and extracted with ethyl acetate. The combined organic layers were washed with water, and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solution was filtered through a Celite pad, and the filtrate was concentrated by evaporation. The crude product of **5b** was used in the next reaction.

To a solution of **5b** (3.00 g, 8.08 mmol) and spiro[2,7-dimethylacridan-9,9'-fluorene] (2.91 g, 8.10 mmol) in dry toluene (100 mL) were added Pd(OAc)<sub>2</sub> (0.05 g, 0.22 mmol), P(*t*-Bu)<sub>3</sub>HBF<sub>4</sub> (0.35 g, 1.21 mmol) and *t*-BuONa (1.86 g, 19.4 mmol). The mixture was refluxed for 24 h under N<sub>2</sub>. After cooling to room temperature, the reaction mixture was poured into water and then extracted with CHCl<sub>3</sub>. The combined organic layers were washed with water and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After filtration and evaporation, the product was purified by column chromatography on silica gel (eluent: CH<sub>2</sub>Cl<sub>2</sub>), recrystallized from CH<sub>2</sub>Cl<sub>2</sub>/hexane, and dried under vacuum to afford MFAc-OPO as a light yellow solid (yield = 2.56 g, 23%). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.05 (d,  $J$  = 8.4 Hz, 0.5H), 8.02 (d,  $J$  = 8.4 Hz, 0.5H), 7.97 (d,  $J$  = 7.6 Hz, 2H), 7.81–7.67 (m, 5H), 7.63–7.55 (m, 4H), 7.51 (d,  $J$  = 8.4 Hz, 1H), 7.43 (td,  $J$  = 7.2 Hz, 1.2 Hz, 3H), 7.37 (d,  $J$  = 6.8 Hz, 2H), 7.31 (td,  $J$  = 7.6 Hz, 1.2 Hz, 2H), 6.79 (dd,  $J$  = 8.4 Hz, 2.0 Hz, 2H), 6.29 (d,  $J$  = 8.4 Hz, 2H), 6.03 (d,  $J$  = 2.0 Hz, 2H), 1.88 (s, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 157.70 (d,  $J_{CP}$  = 3.7 Hz), 156.23, 155.75, 147.02, 139.30, 138.61, 134.14, 134.02 (d,  $J_{CP}$  = 5.3 Hz), 133.11, 132.11, 131.85 (d,  $J_{CP}$  = 10.8 Hz), 131.47 (d,  $J_{CP}$  = 5.3 Hz), 130.12, 128.75 (d,  $J_{CP}$  = 12.8 Hz), 128.39, 128.05 (d,  $J_{CP}$  = 3.5 Hz), 127.56, 127.20 (d,  $J_{CP}$  = 10.8 Hz), 125.75, 124.95, 124.54 (d,  $J_{CP}$  = 10.8 Hz), 121.24 (d,  $J_{CP}$  = 6.3 Hz), 119.90, 118.46

(d,  $J_{CP} = 5.7$  Hz), 115.90 (d,  $J_{CP} = 30.8$  Hz), 115.08 (d,  $J_{CP} = 32.5$  Hz), 114.46, 56.81, 20.40. MS (MALDI-TOF):  $m/z$  calcd 649.22 [ $M$ ]<sup>+</sup>; found, 649.12. Anal. calcd (%) for C<sub>38</sub>H<sub>25</sub>NO<sub>2</sub>: C 83.19, H 4.96, N 2.16; found: C 82.63, H 4.99, N 2.18.

**Synthesis of MFAc-OPS (3).** A mixture of MFAc-OPO (1.00 g, 1.54 mmol) and Lawesson's reagent (1.25 g, 3.09 mmol) in dry toluene (100 mL) was refluxed for 24 h under N<sub>2</sub>. After cooling to room temperature, the solvent was removed under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: hexane/CHCl<sub>3</sub> = 3/1, v/v), and recrystallized from CH<sub>2</sub>Cl<sub>2</sub>/hexane, and dried under vacuum to afford MFAc-OPS as a light yellow solid (yield = 0.76 g, 75%). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  8.18 (d,  $J = 8.4$  Hz, 0.5H), 8.14 (d,  $J = 8.4$  Hz, 0.5H), 7.97 (d,  $J = 7.2$  Hz, 2H), 7.89 (dd,  $J = 7.6$  Hz, 1.6 Hz, 0.5H), 7.85 (dd,  $J = 7.6$  Hz, 1.6 Hz, 0.5H), 7.79–7.72 (m, 4H), 7.58–7.56 (m, 4H), 7.53–7.41 (m, 4H), 7.37 (d,  $J = 7.2$  Hz, 2H), 7.30 (td,  $J = 7.2$  Hz, 0.8 Hz, 2H), 6.79 (dd,  $J = 8.4$  Hz, 2.0 Hz, 2H), 6.28 (d,  $J = 8.4$  Hz, 2H), 6.03 (d,  $J = 2.0$  Hz, 2H), 1.88 (s, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  156.42 (d,  $J_{CP} = 2.3$  Hz), 156.19, 154.53, 146.61 (d,  $J_{CP} = 2.6$  Hz), 139.28, 138.57, 135.90, 135.19, 134.55 (d,  $J_{CP} = 8.4$  Hz), 133.73, 132.00 (d,  $J_{CP} = 8.0$  Hz), 131.58 (d,  $J_{CP} = 2.7$  Hz), 131.13 (d,  $J_{CP} = 11.9$  Hz), 130.10, 128.72 (d,  $J_{CP} = 13.2$  Hz), 128.38, 128.21 (d,  $J_{CP} = 5.9$  Hz), 127.74 (d,  $J_{CP} = 11.8$  Hz), 127.55, 125.73, 125.13 (d,  $J_{CP} = 11.7$  Hz), 124.95, 120.92 (d,  $J_{CP} = 6.2$  Hz), 119.90, 118.19 (d,  $J_{CP} = 5.8$  Hz), 115.96 (d,  $J_{CP} = 55.8$  Hz), 115.27 (d,  $J_{CP} = 56.9$  Hz), 114.45, 56.79, 20.39. MS (MALDI-TOF):  $m/z$  calcd 655.19 [ $M$ ]<sup>+</sup>; found, 665.21. Anal. calcd (%) for C<sub>38</sub>H<sub>25</sub>NO<sub>2</sub>: C 81.18, H 4.84, N 2.10; found: C 81.17, H 4.81, N 2.16.

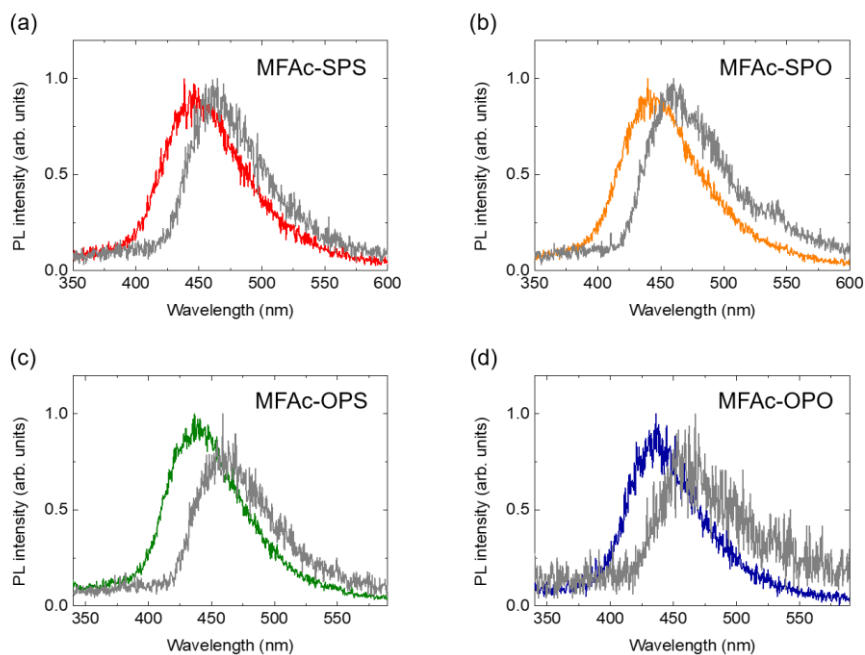


**Fig. S1** TGA curves of **1–4** at a heating rate of  $20\text{ }^{\circ}\text{C min}^{-1}$  under  $\text{N}_2$ .

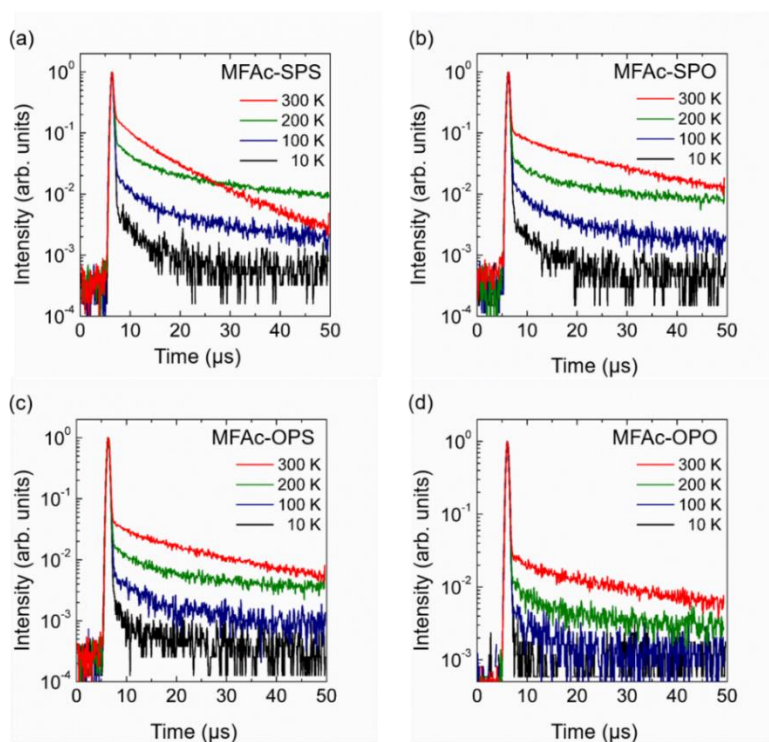
**Table S1** PL properties of **1–4** in toluene solution ( $1 \times 10^{-5}\text{ M}$ )

emitter	in aerated solution			after $\text{N}_2$ bubbling		
	$\Phi_{\text{PL}}^a$ (%)	$\tau_p^b$ (ns)	$\tau_d^c$ ( $\mu\text{s}$ )	$\Phi_{\text{PL}}^a$ (%)	$\tau_p^b$ (ns)	$\tau_d^c$ ( $\mu\text{s}$ )
MFAC-SPS	13	8.4	n.d.	45	12	3.5
MFAC-SPO	13	9.0	n.d.	40	12	3.8
MFAC-OPS	18	10	n.d.	49	16	3.2
MFAC-OPO	18	11	n.d.	49	17	3.3

<sup>a</sup>Absolute PL quantum yield evaluated using an integrating sphere at 300 K. <sup>b</sup>Lifetime for prompt fluorescence. <sup>c</sup>Lifetime for delayed fluorescence.

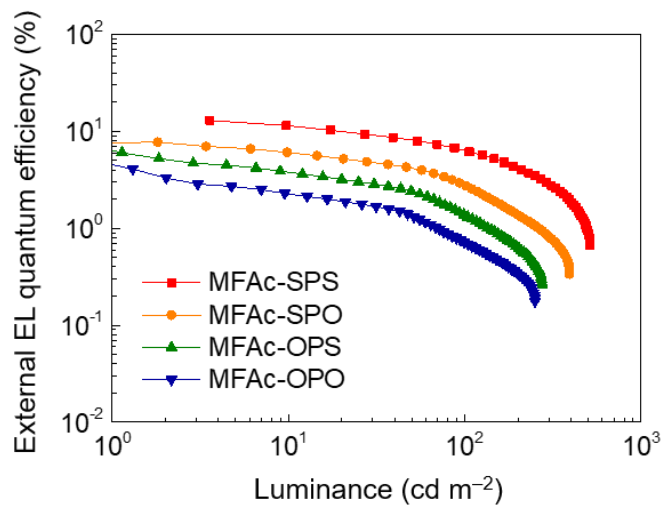


**Fig. S2** Fluorescence spectra in the range of 1–100 ns (colored lines) and phosphorescence spectra in the range of 1–10 ms (gray lines) at 10 K for (a) 20 wt%-1:PPF, (b) 20 wt%-2:PPF, (c) 20 wt%-3:PPF and (d) 20 wt%-4:PPF doped films.



**Fig. S3** Temperature dependence of transient PL decays ranging from 10 to 300 K for (a) 20 wt%-1:PPF, (b) 20wt%-2:PPF, (c) 20wt%-3:PPF and (d) 20 wt%-4:PPF doped films.



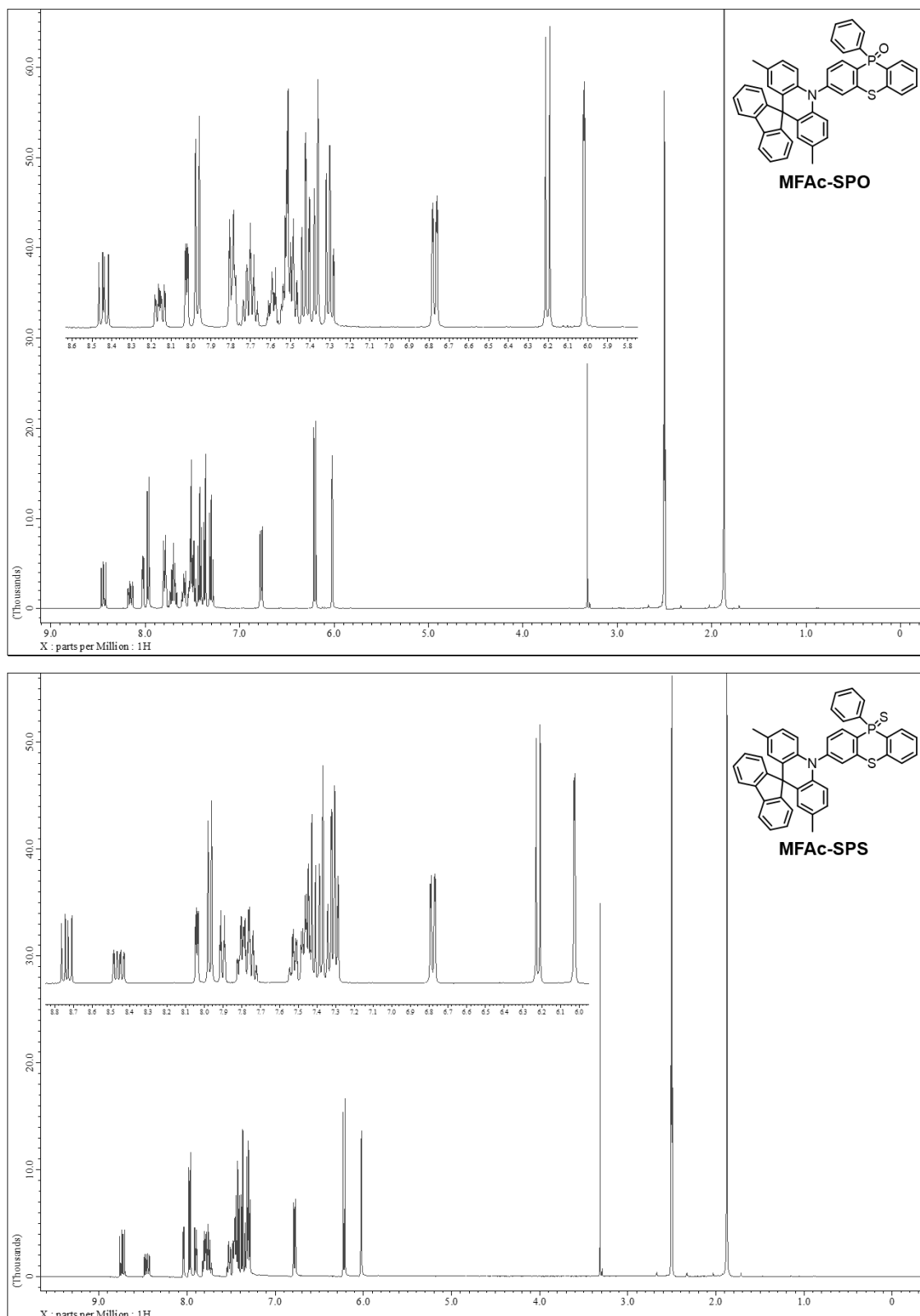


**Fig. S4** External EL quantum efficiency vs. luminance ( $\eta_{\text{ext}}-L$ ) characteristics for blue TADF-OLEDs.

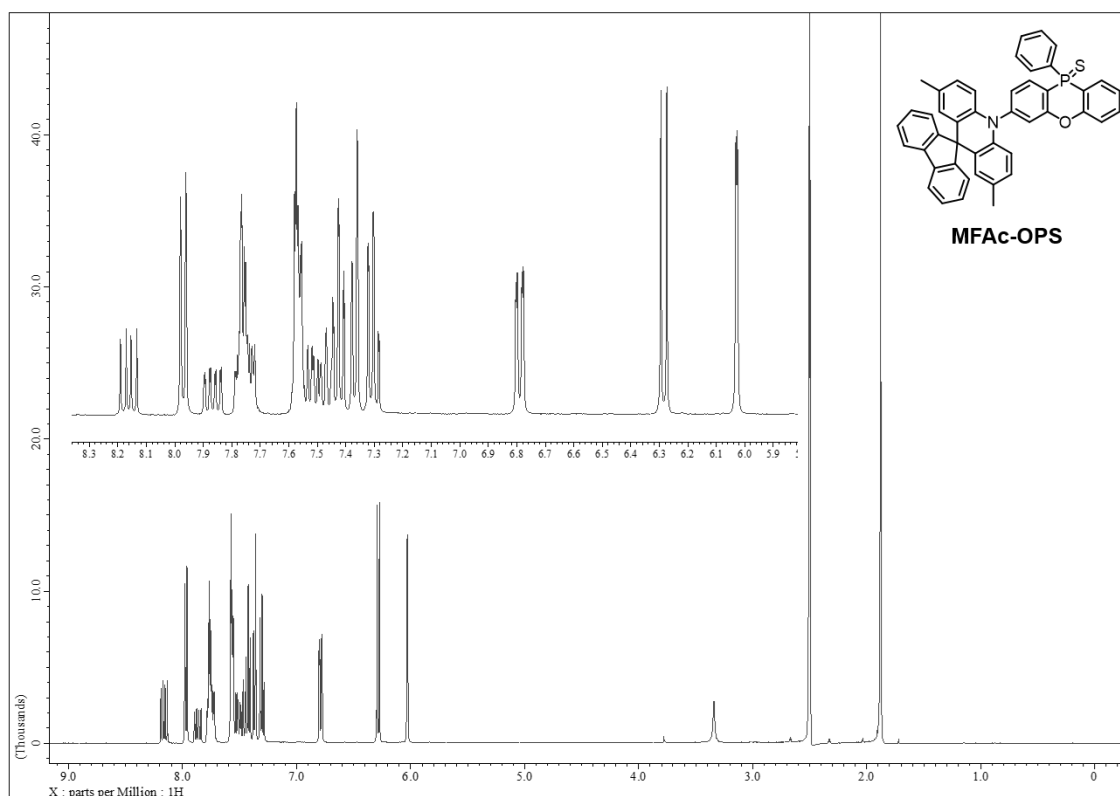
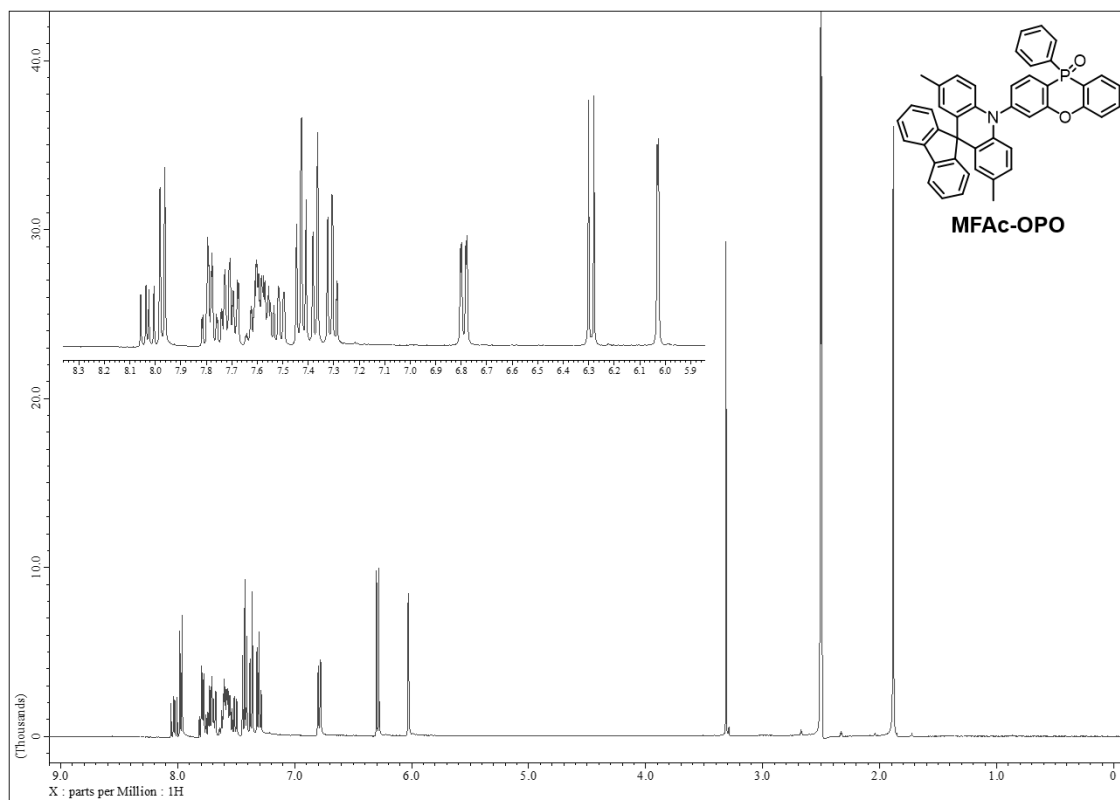
**Table S2** EL performances of TADF-OLEDs based on **1–4**

emitter	$\lambda_{\text{EL}}^a$ (nm)	$V_{\text{on}}^b$ (V)	$\eta_{\text{ext}}^c$ (%)	$\eta_c^d$ (cd A <sup>-1</sup> )	$\eta_p^e$ (lm W <sup>-1</sup> )	CIE <sup>f</sup> (x, y)
MFAc-SPS	473	3.0	13.0	21.6	22.6	(0.16, 0.23)
MFAc-SPO	468	3.0	7.7	11.6	12.0	(0.16, 0.19)
MFAc-OPS	462	3.2	7.5	9.7	9.5	(0.16, 0.16)
MFAc-OPO	461	3.0	4.9	6.4	6.7	(0.16, 0.15)

<sup>a</sup>EL emission maximum. <sup>b</sup>Turn-on voltage at 1 cd m<sup>-2</sup>. <sup>c</sup>Maximum external EL quantum efficiency. <sup>d</sup>Maximum current efficiency. <sup>e</sup>Maximum power efficiency. <sup>f</sup>Commission Internationale de l'Éclairage color coordinates measured at 10 mA cm<sup>-2</sup>.



**Fig. S5**  $^1\text{H}$  NMR spectra of MFAc-SPO and MFAc-SPS in  $\text{DMSO-}d_6$ .



**Fig. S6**  $^1\text{H}$  NMR spectra of MFAc-OPO and MFAc-OPS in  $\text{DMSO-}d_6$ .

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