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Supporting Information(SI)

Synthesis and Aggregation induced emission property of novel boron-containing derivatives with Sensors for Viscous Alcohol-Fluids

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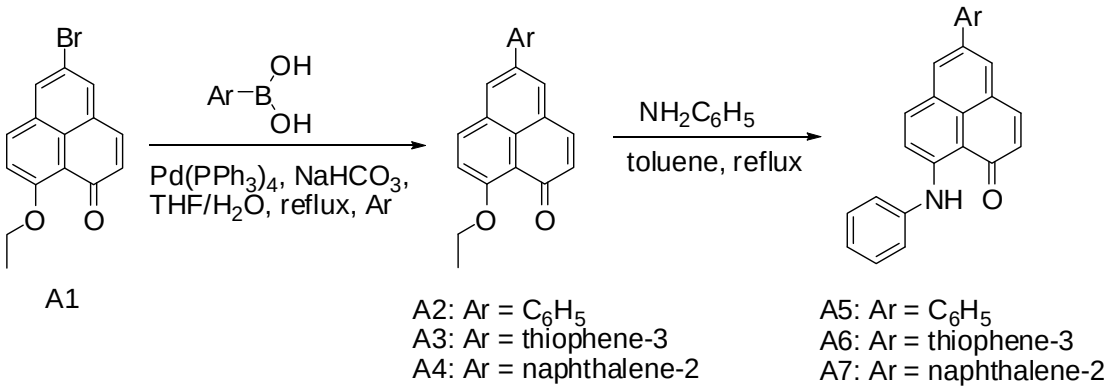
Synthesis



Scheme S1. The procedure for synthesis of compound **A3** and **A5-A7**.

The procedures for synthesis of compound **A1, A2** and **A4** were according to the literatures [1].

Synthesis of compound A3

Compound 5-Bromo-9-ethoxy-1-oxophenalene, **A1** (1.82 g, 6.0 mmol), 3-thiopheneboronic acid (0.92 g, 7.2 mmol), $Pd(PPh_3)_4$ (0.21 g, 0.18 mmol), $NaHCO_3$ (1.51 g, 18 mmol) was added into degassed THF (50 mL)/water (30 mL) under argon. Then the mixture was refluxed at 90 ^oC for 48

hours. After the solution cooled down, the mixture was extracted by CH_2Cl_2, and then obtained organic phase was washed by saturated aqueous NH_4Cl and dried by anhydrous Na_2SO_4. Then it was filtrated and concentrated to obtained crude product, which was purified (silica gel, petroleum ether/ethyl acetate 3:1, v/v) to give **A3** (1.38 g, 4.50 mmol) as a yellow powder, yield: 75.0 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ [ppm] = 8.19 (1H, d, *J* = 9.2 Hz), 8.13 (1H, d, *J* = 1.6 Hz), 8.03 (1H, d, *J* = 1.6 Hz), 7.73 (1H, d, *J* = 9.2 Hz), 7.61 (1H, q, *J* = 1.6 Hz), 7.53 (1H, q, *J* = 1.6 Hz), 7.50-7.47 (2H, m), 6.78 (1H, d, *J* = 9.6 Hz), 4.45 (2H, q, *J* = 7.2 Hz), 1.65 (3H, t, *J* = 7.2 Hz).

Synthesis of compound A5

Compound **A2** (1.20 g, 4.0 mmol) and aniline (0.75 g, 8.0 mmol) was added in toluene (30 mL) and stirred and refluxed at 120 ^{o}C for 12 hours. Then the mixture was cooled down and excess solvent was removed to obtain crude product, which was purified (silica gel, petroleum ether/ethyl acetate 10:1, v/v) to give **A5** (1.26 g, 3.64 mmol) as a red powder, yield: 91.0 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ [ppm] = 13.75 (1H, s), 8.11 (2H, d, *J* = 3.6 Hz), 7.97 (1H, d, *J* = 7.2 Hz), 7.94 (1H, d, *J* = 7.2 Hz), 7.73 (2H, d, *J* = 7.6 Hz), 7.54-7.45 (5H, m), 7.42-7.38 (3H, m), 7.30 (1H, t, *J* = 9.2 Hz), 7.05 (1H, d, *J* = 7.2 Hz). MS (ESI): calcd. for M = $[C_{25}H_{17}ON]$: 347.4; found: $[M+1]^+$: 348.1.

Synthesis of compound A6

The method to synthesize compound **A6** is similar with that of **A5.** Yield: 92.5 %.

^{1}H NMR (300 MHz, $CDCl_3$): δ [ppm] = 13.02 (1H, s), 8.25 (2H, d, *J* = 14.4 Hz), 8.15 (1H, d, *J* = 9.3 Hz), 8.07 (1H, d, *J* = 9.6 Hz), 7.75 (1H, d, *J* = 9.3 Hz), 7.40-7.63 (1H, m), 7.56-7.49 (4H, m), 7.46-7.41 (4H, m). MS (ESI): calcd. for M = $[C_{23}H_{15}SON]$: 353.4; found: $[M+1]^+$: 354.1.

Synthesis of compound A7

The method to synthesize compound **A6** is similar with that of **A5.** Yield: 85.8 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ [ppm] = 13.75 (1H, s), 8.21 (2H, d, *J* = 3.6 Hz), 8.15 (1H, m), 8.00-7.84 (6H, m), 7.54-7.39 (7H, m), 7.29 (1H, t, *J* = 9.6 Hz), 7.06 (1H, d, *J* = 12.4 Hz). MS (ESI): calcd for: M = $[C_{29}H_{19}ON]$: 397.5; found: $[M+1]^+$: 398.2.

Calculation analysis

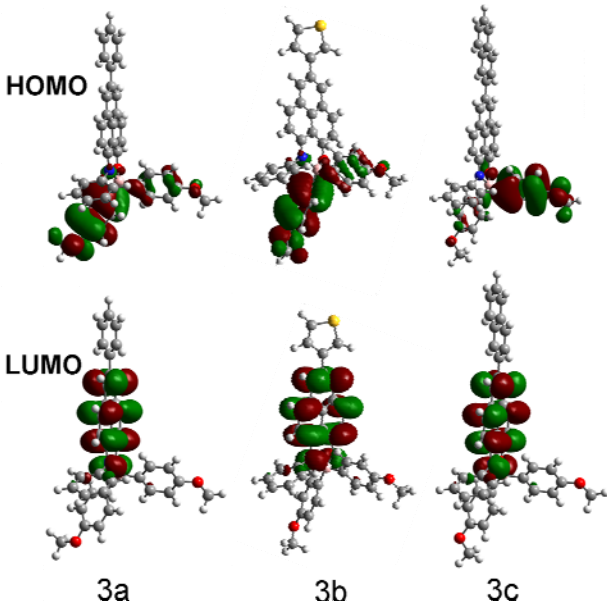


Figure S1. A) Optimized molecular structures, and molecular orbital amplitude plots of HOMOs and LUMOs of compounds **3(a,b,c)** calculated using B3LYP/6-31G*.

Spectroscopic properties

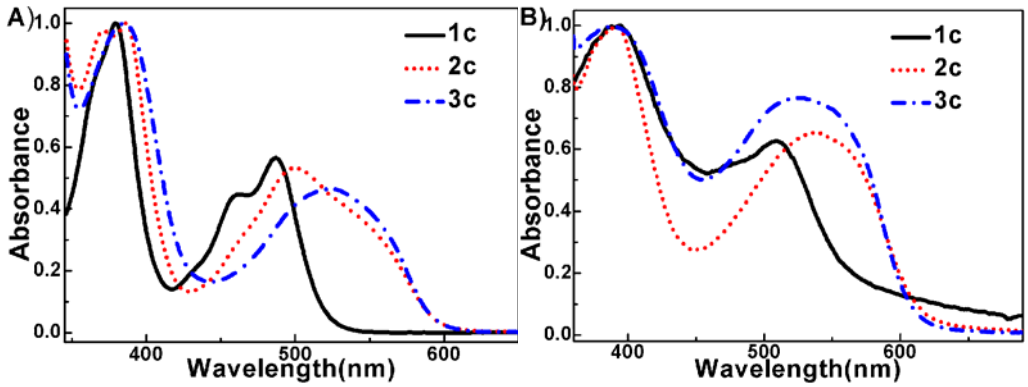


Figure S2. A) Absorption spectra of **1c**, **2c** and **3c** in THF solutions; B) Absorption spectra of **1c**, **2c** and **3c** in solid film.

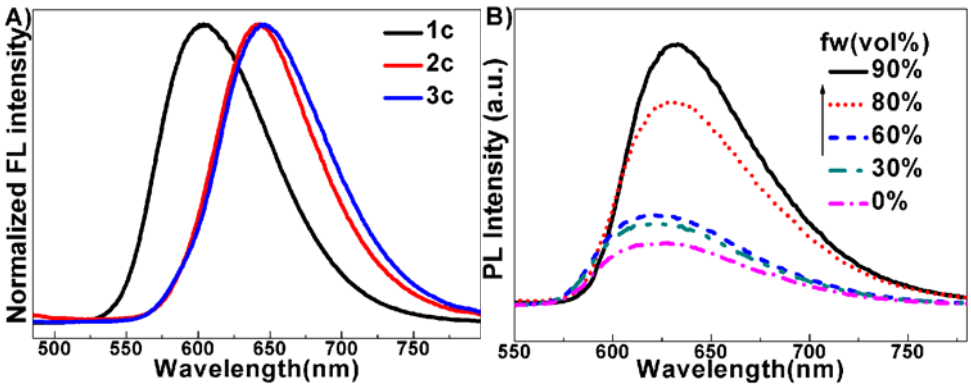


Figure S3. A) PL spectra of **1c-3c** in solid film, excited at maximum excitation wavelength, 395 nm. B) PL spectra of **3b** in THF/water mixtures with different water fraction (fw), excited at 468 nm.

Electrochemical analysis

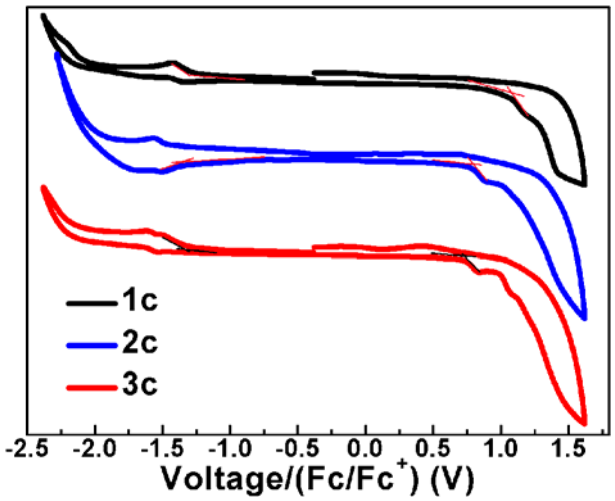


Figure S4. Cyclic voltammograms of **1c-3c** in a dichloromethane solution of 0.1 $molL^{-1}$ Bu_4NPF_6 with a scan rate of 0.1 $Vs^{-1}$and Fc/Fc^+ as internal reference.

Optical and electrochemistry data

Table S1. Optical and electrochemistry data summary of compound **1a-3c.**

Compound	λ_{abs}^{max}(nm) Solution[a]	λ_{abs}^{max}(nm) Film[b]	λ_{FL}^{max}(nm) Film[c]	HOMO[d] (ev)	LUMO[d] (ev)	Eg_{cv}^{d} (ev)	Eg_{opt}^{d} (ev)	Φ_F(%) Film
1a	377,483	387,500	579	-6.05	-3.52	2.53	2.42	38
1b	380,491	379,483	593	-5.86	-3.49	2.37	2.38	34
1c	379,487	390,509	603	-5.89	-3.50	2.39	2.39	17
2a	386,520	394,538	645	-5.26	-3.27	1.99	2.11	74
2b	387,503	399,543	635	-5.55	-3.51	2.04	2.08	69
2c	386,500	391,537	643	-5.52	-3.50	2.20	2.09	73
3a	383,506	388,525	644	-5.35	-3.34	2.01	2.10	81
3b	382,502	390,533	636	-5.52	-3.50	2.02	2.07	70
3c	385,523	389,525	646	-5.54	-3.47	2.07	2.09	67

[a] In THF solution (10 μm). [b] Film drop-casted on quartz plate. [c] Film drop-casted on quartz plate.

[d] HOMO (/Fc) = -e (E^1, ox) + (-4.8) eV, LUMO (/Fc) = -e (E^1, re) + (-4.8) eV, $E_{g/cv}$ = LUMO-HOMO, $E_{g/opt} = 1240 / \lambda_g$.

Reference

1 W. Yan, C. Hong, G. Long, Y. Yang, Z. Liu, Z. Bian, Y. Chen, C. Huang, Dyes Pigments 106 (2014) 197-204.