

Instruments and methods

¹H NMR spectra were recorded on a VNMRS 400 NMR spectrometer (Varian, USA). High resolution mass spectra (HR-MS) were recorded using an Autoflex III mass spectrometer (MALDI-TOF-MS, Bruker, Germany). TGA analysis was performed on a NETZSCH SA409PC thermogravimeter. DSC measurements were carried out on a NETZSCH DSC 200F3 instrument at a heating rate and a cooling rate of 10 °C min⁻¹ in nitrogen. UV-Vis spectra were recorded using a UV-2600 spectrometer (Shimadzu, Japan). Fluorescence spectra were recorded using a F-7000 fluorescence spectrometer (Hitachi, Japan). Absolute quantum efficiency was measured on an integrating sphere (C11347-11, Hamamatsu, Japan). Fluorescence lifetime was measured on a compact fluorescence lifetime spectrometer (C11367-11, Hamamatsu, Japan). Powder X-ray diffraction (PXRD) patterns were carried out in the reflection mode at room temperature using a 2.2 kW Empyrean X-ray Diffraction System (PANalytical, Netherland). The ML spectra were collected from a spectrometer of Acton SP2750 with a liquid-nitrogen-cooled CCD (SPEC-10, Princeton) as a power detector (data-collection time is 1s and the diameter of optical fiber is 600 μm). The theoretical ground-state geometry and electronic structure of molecule was optimized using the density functional theory (DFT) with B3LYP hybrid functional at the basis set level of 6-31+G(d). All the theoretical calculations were performed using Gaussian 03 package.¹

*Preparation of 1.*² 1-(4-Bromophenyl)-1,2,2-triphenylethylene (1 g, 2.43 mmol) was firstly placed in a 50 mL round bottom flask. The flask was evacuated under vacuum and flushed with nitrogen three times. THF (20 mL) was then added. The mixture was cooled to -78 °C and n-BuLi (2.5 M, 1.17 mL, 2.92 mmol) was slowly added. After the mixture was stirred for 3 h at -78 °C, trimethyl borate (542 μL, 4.86 mmol) was injected. After 3 h, the mixture was slowly warmed to room temperature. HCl (2 M, 10 mL) solution was added and the mixture was stirred for another 3 h. Then the reaction mixture was diluted with CH₂Cl₂, washed with water and brine, dried over Na₂SO₄. The solvents were removed under reduced pressure. The residue was purified

by chromatography on a silica gel column (DCM/EtOAc = 4/1, v/v) to yield the compound **1** (383 mg, 42.1%) as white powder. ^1H NMR (400 MHz, DMSO- d_6): δ = 7.94 (s, 2H), 7.53 (d, J = 8.0 Hz, 2H), 7.07-7.16 (m, 9H), 6.92-6.99 ppm (m, 8H); ^{13}C NMR (100 MHz, DMSO- d_6): δ = 144.88, 143.18, 143.15, 140.67, 133.62, 130.65, 129.69, 127.83, 126.59, 126.56 ppm; element analysis calcd. (%) for $\text{C}_{26}\text{H}_{21}\text{BO}_2$: C 83.00; H 5.63; found: C 83.42; H 5.52.

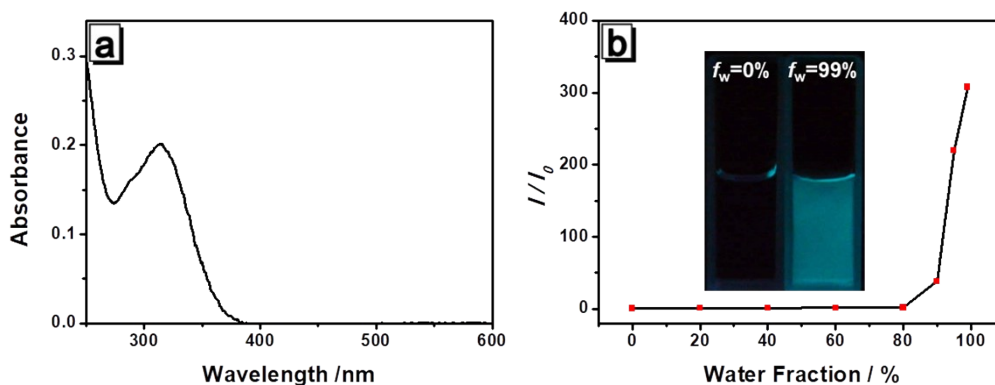


Figure S1. (a) Absorption of **1** in THF solution (10 μM). (b) Plots of I/I_0 versus water fractions of **1**, where I_0 is the emission intensity at 460 nm in THF (10 μM). Inset: fluorescence images at $f_w = 0\%$ and 99%.

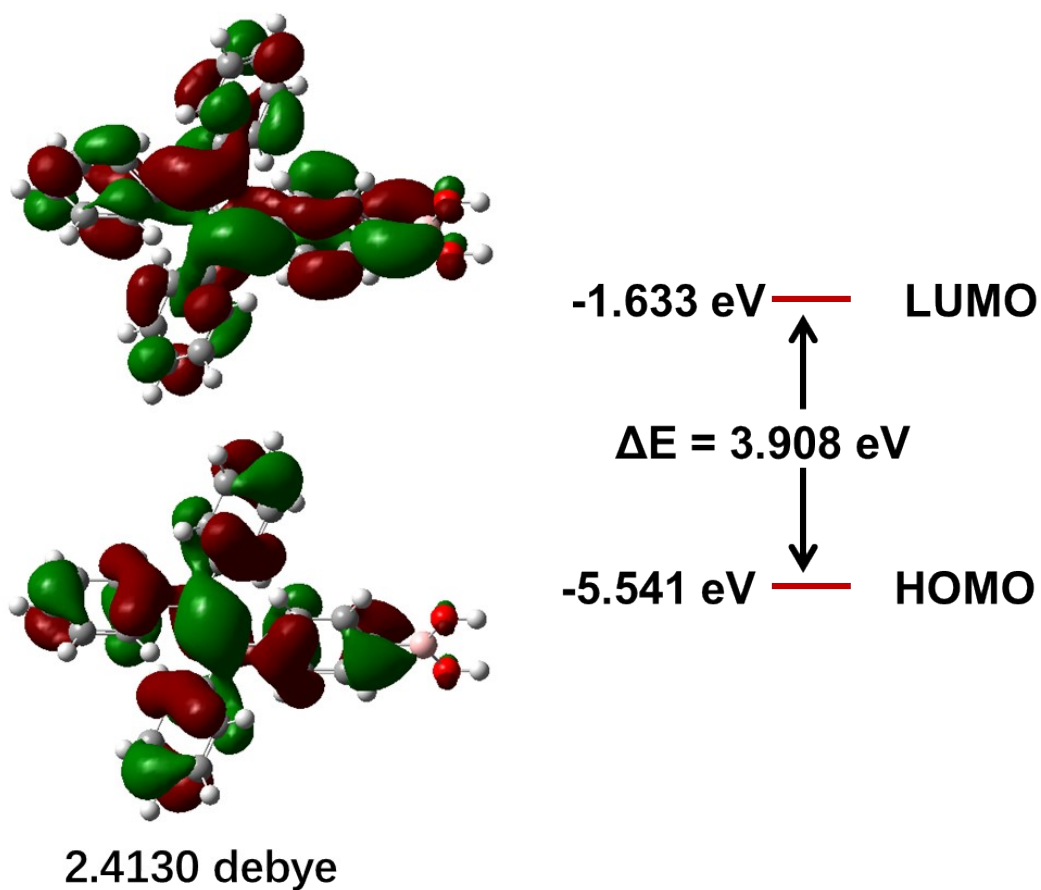


Figure S2. The HOMO and LUMO orbital distribution of **1** calculated by B3LYP/6-31+G(d).

Table S1. Optical properties of compound **1** in various solid forms.

	$\lambda_{em}[nm]^a$	$\Phi_f[\%]^b$	$\tau[ns]^c$
1o	460	— ^d	— ^d
1g	490	50.9	3.323
1f	449	48.1	2.545
1h	465	52.0	3.038

^aEmission maximum. ^bFluorescence quantum yield determined by using a calibrated integrating sphere. ^cFluorescence lifetime. ^dNot determined.

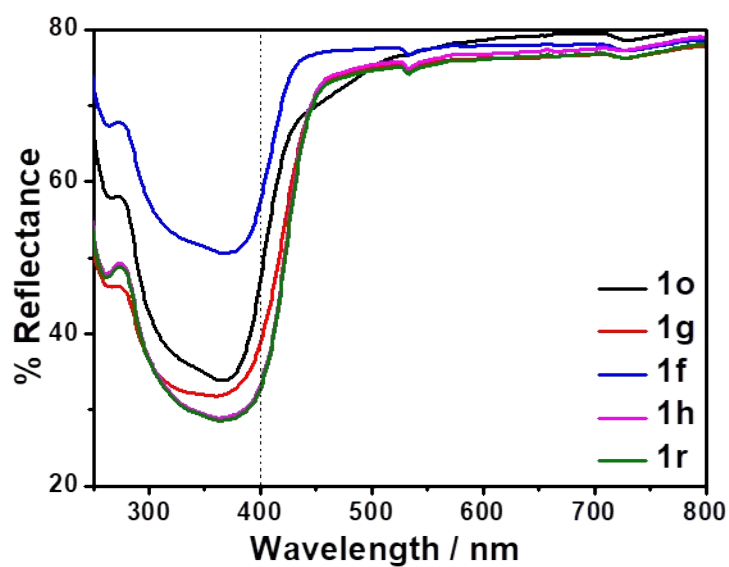


Figure S3. UV-Vis reflection spectra of different states of **1**.

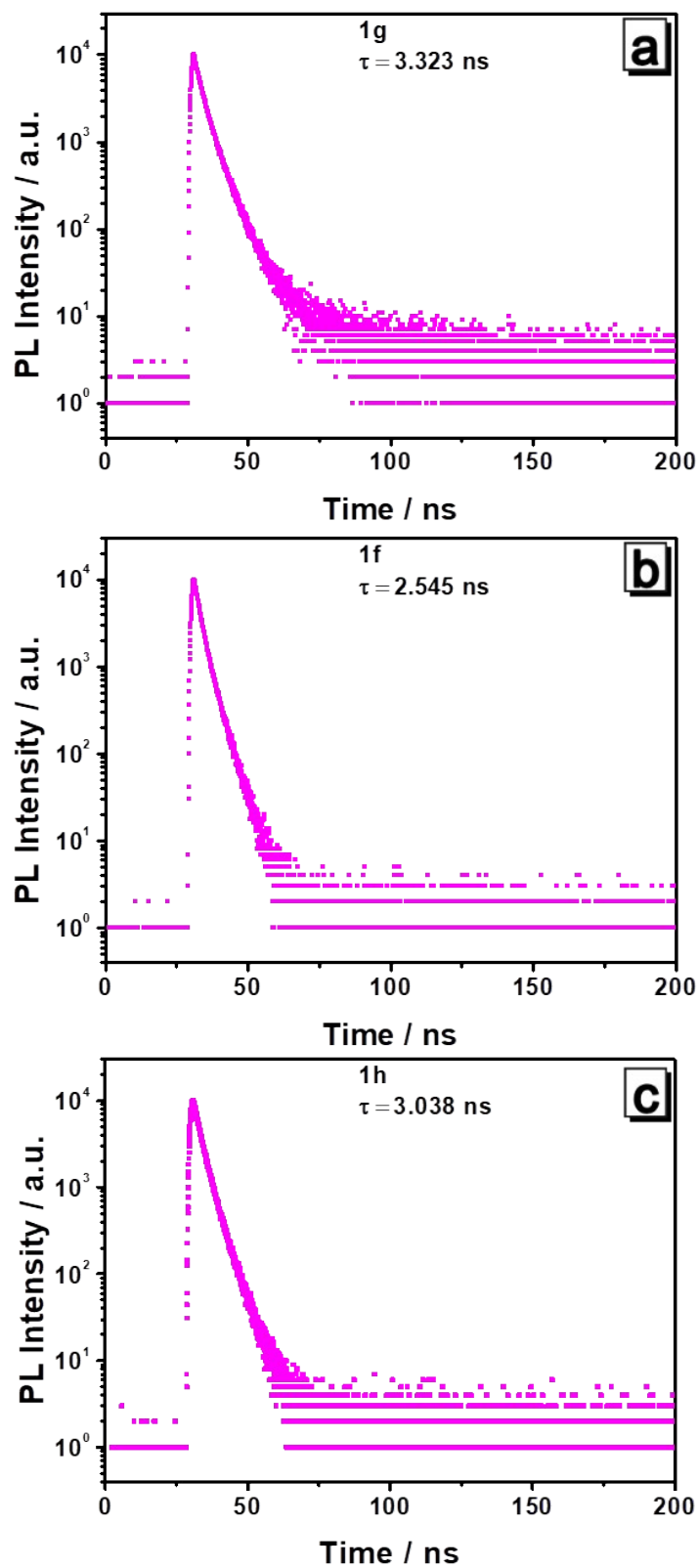


Figure S4. Fluorescence decay curves of ground powder (**1g**), fumed powder (**1f**) and heated powder (**1h**) of **1**.

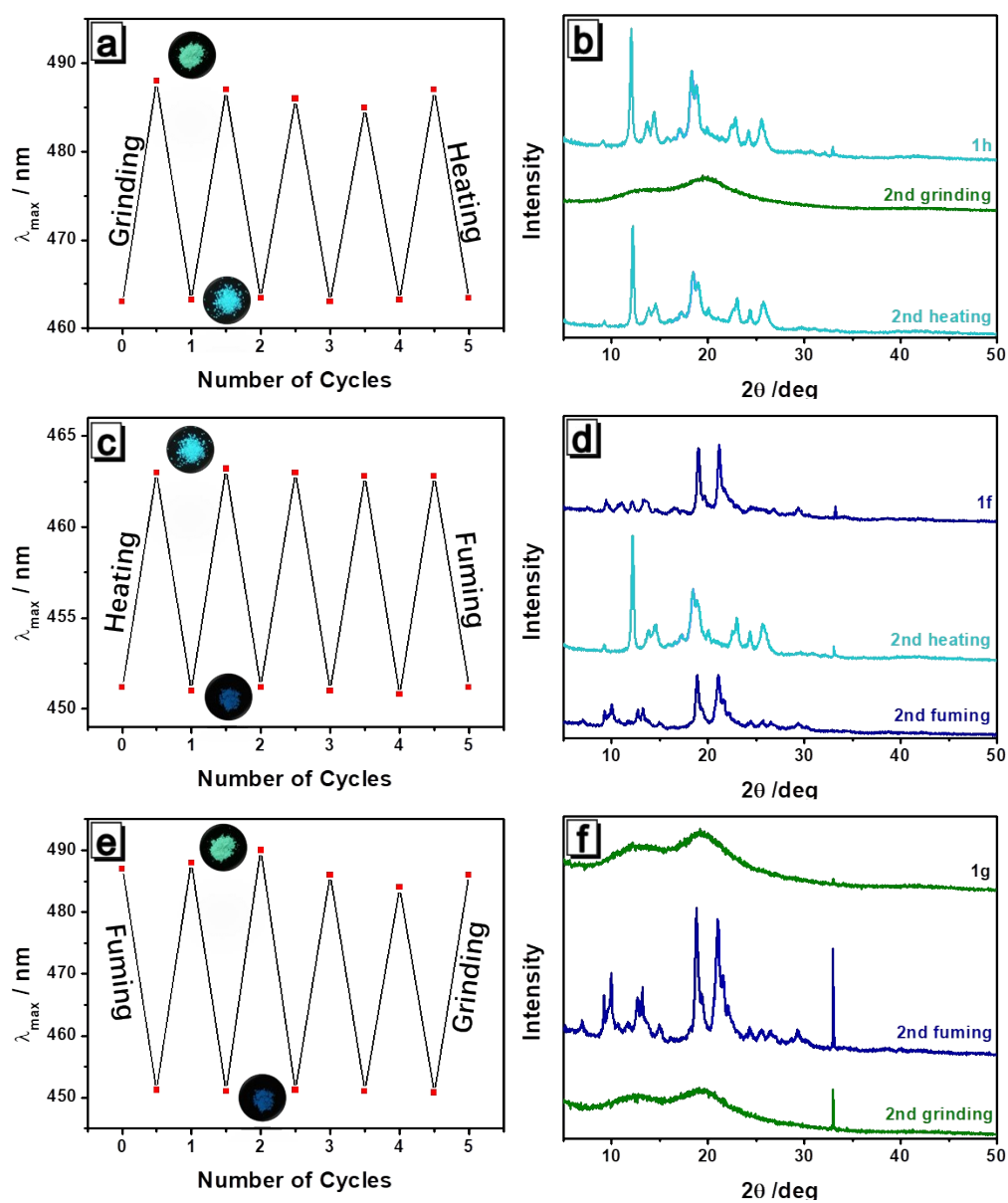


Figure S5. Maximum emission wavelength changes of **1** cast weighing paper versus (a) grinding/heating, (c) heating/methanol fuming and (e) methanol fuming /grinding cycles. PXRD patterns of **1** during (b) grinding/heating, (d) heating/methanol fuming and (f) methanol fuming /grinding cycles.

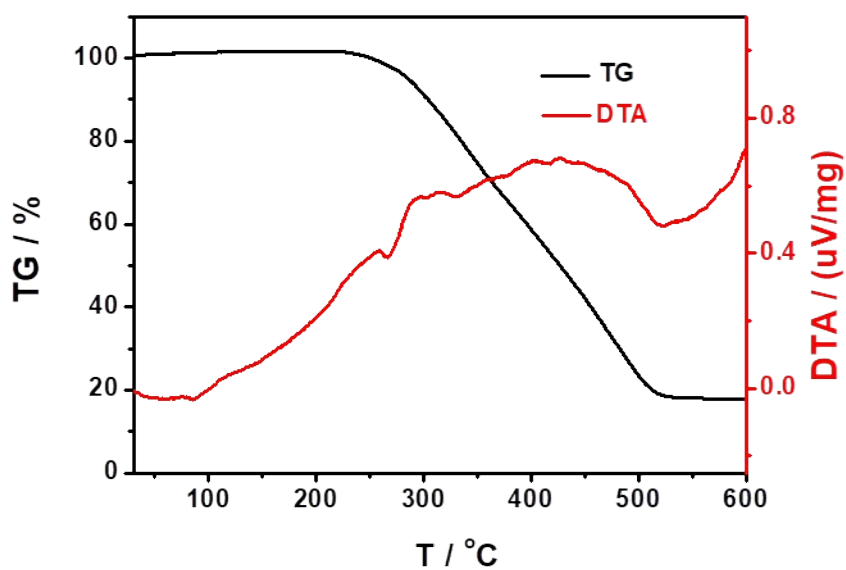


Figure S6. TG and DTA curves of **1** measured at a heating rate of 10 $^\circ\text{C}/\text{min}$ under nitrogen atmosphere.

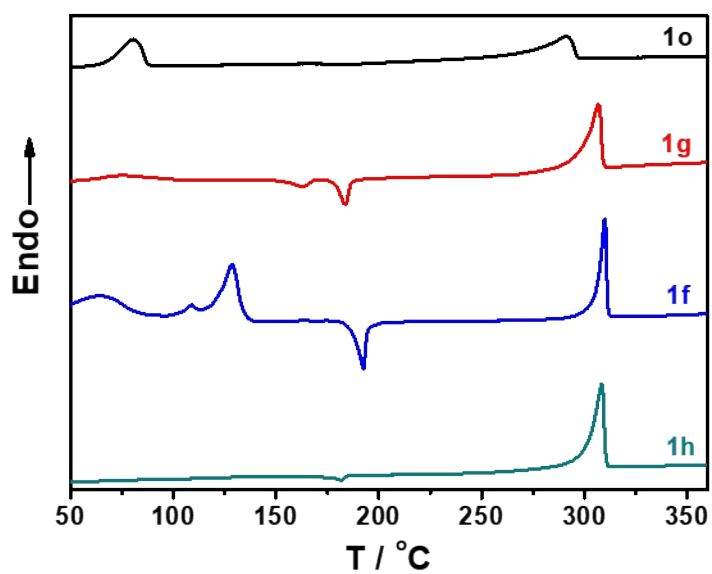


Figure S7. DSC curves of the as-prepared powder (**1o**), ground powder (**1g**), fumed powder (**1f**) and heated powder (**1h**).

Table S2. Single crystal data of **1c**.

CCDC number	2084062
Formula	$C_{27.5}H_{24}BO_{2.75}$
Formula weight /g•mol ⁻¹	409.28
Crystal system	monoclinic
Space group	C2/c
T/K	100
Z	16
a/Å	49.972(3)
b/Å	5.4225(3)
c/Å	36.9982(19)
$\alpha/^\circ$	90
$\beta/^\circ$	110.411(3)
$\gamma/^\circ$	90
V/Å ³	9396.1(9)
$\rho_c/g\cdot cm^{-3}$	1.157
μ/mm^{-1}	0.573
F(000)	3456.0
Reflections collected	80586
Independent reflections	8630
R _{int}	0.0704
R ₁ (I > 2 σ (I))	0.1059
wR ₂	0.3177
GOOF	1.050

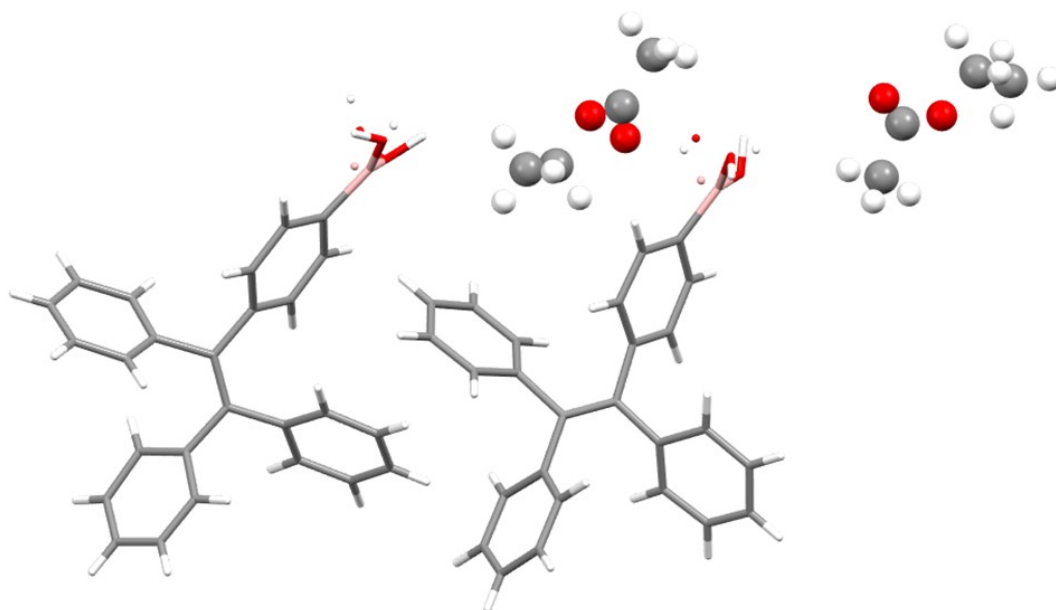


Figure S8. Two kinds of molecular conformations in single crystal **1c**. Every boric acid group in one molecule has two possible positions by virtue of disorder distribution.

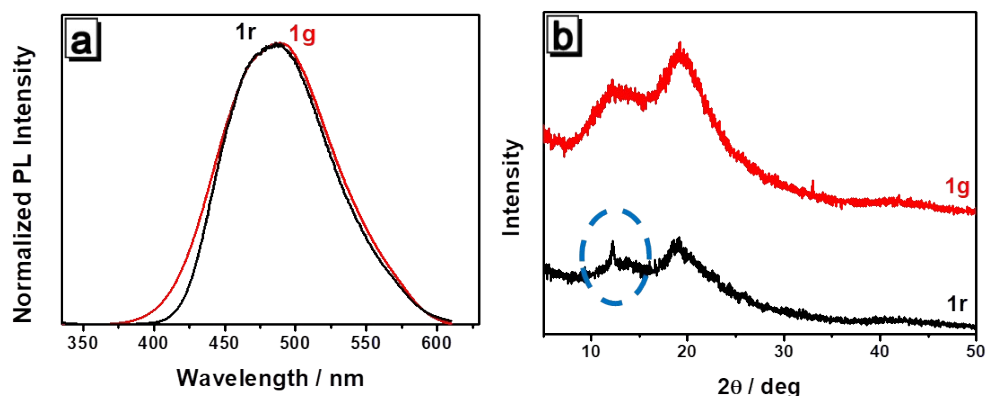


Figure S9. (a) Normalized fluorescence spectra and (b) PXRD patterns of **1g** and **1r**.

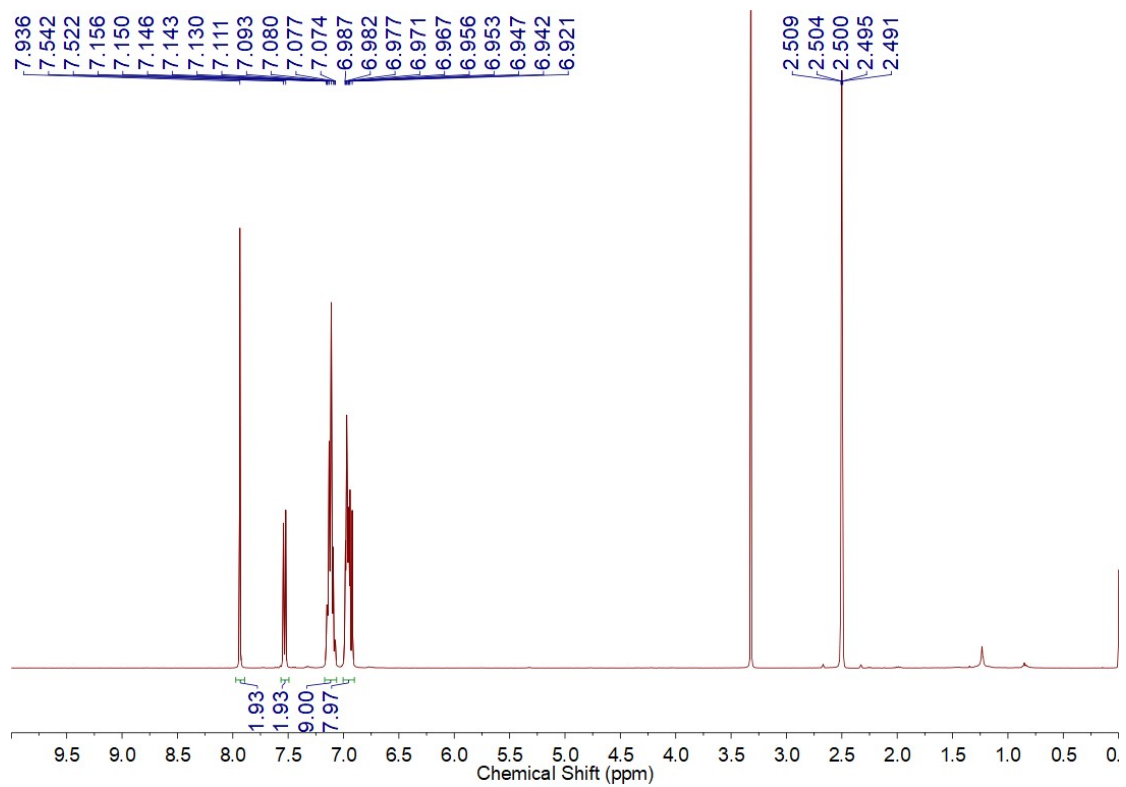


Figure S10. ^1H NMR of compound **1**.

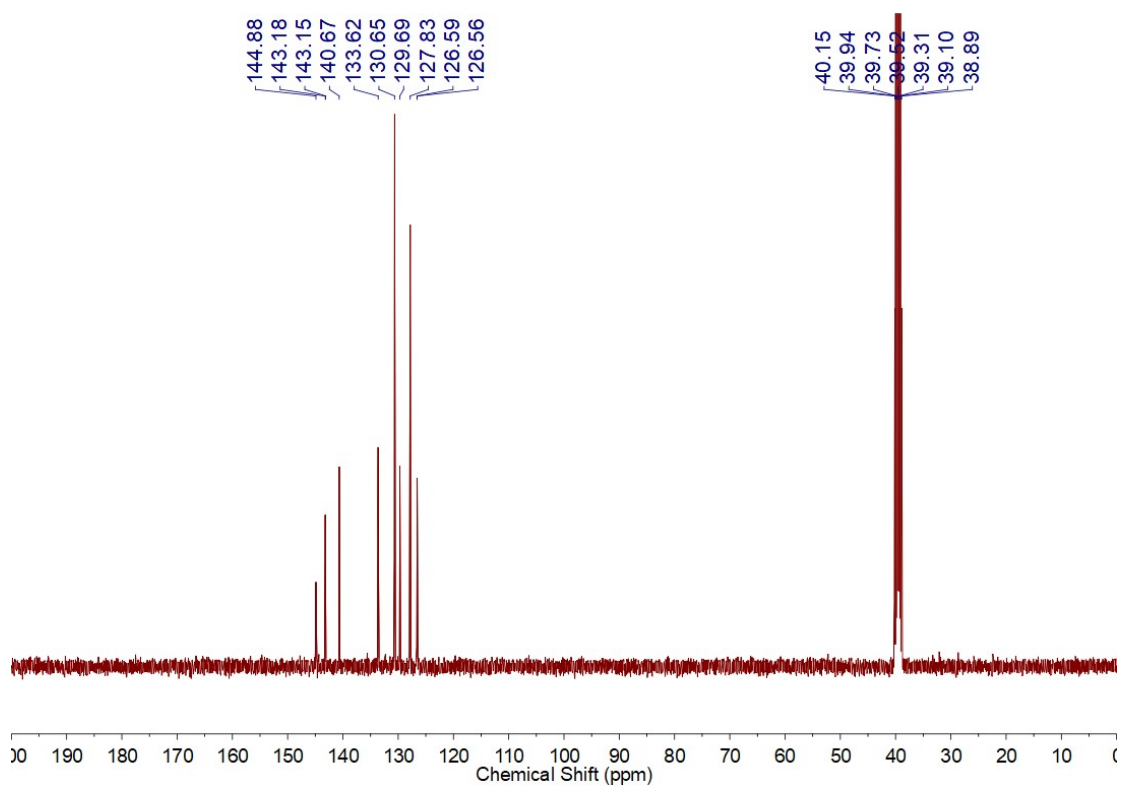


Figure S11. ^{13}C NMR of compound **1**.

Reference

1. Gaussian 03, Revision E.01, M. J. Frisch et al., Gaussian, Inc., Wallingford CT, 2009.
2. Yuan, W. Z.; Lu, P.; Chen, S.; Lam, J. W. Y.; Wang, Z.; Liu, Y.; Kwok, G. S.; Ma, Y.; Tang, B. Z. *Adv. Mater.* **2010**, *22*, 2159–2163.