Supporting Information

Salicylaldimine Difluoroboron Complexes Containing *tert*-Butyl Groups: Nontraditional π -Gelator and Piezofluorochromic Compounds

Peng Gong, Jingbo Sun, Hao Yang, Zhenqi Zhang, Jiabao Sun, Pengchong Xue, Ran Lu*

State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P. R. China E-mail: luran@mail.jlu.edu.cn; Fax: +86-431-88499179

Compound	Solution ^a		Xerogel	As- prepared crystal	Ground powder	Heated sample	Fumed sample ^e
	$\lambda^{abs}_{max} (nm)$ ($\epsilon \ 10^4 L \cdot mol^{-1} \cdot cm^{-1}$)	$\lambda_{em}(nm)$ ($\Phi_F{}^b$ %)	$\lambda_{em}^{c}(nm)$ (Φ_{F} %)	$\lambda_{em}^{d}(nm)$ (Φ_{F} %)	$\lambda_{em}^{d} (nm)$ ($\Phi_{F} \%$)	λ _{em} ^d (nm)	$\lambda_{em}(nm)$
1B	289 (1.9)	458 (19)	445 (13)	-	-	-	-
	355 (0.5)						
2B	326 (2.8)	505 (13)	-	487 (12)	509 (12)	478	-
	403 (1.7)						
3B	311 (3.9)	506 (19)	-	480 (17)	503 (16)	476	475
	396 (1.5)						

Table S1. Photophysical date of 1B-3B.

^a in CH₂Cl₂ (5.0×10^{-6} M); ^b for **1B** using quinine sulfate in 0.1 M H₂SO₄ ($\Phi_F = 54.6\%$) as the standard, for **2B** and **3B**, using 9,10-diphenylanthracene in benzene ($\Phi_F = 85\%$) as the standard; ^c Excited at 288 nm; ^d Excited at 350 nm for **2B** and 407 nm for **3B**; ^e Fumed with CH₂Cl₂.



Figure S1. The optimized configurations for 1B (a), 2B (b) and 3B (c) calculated by the DFT method (B3LYP/6-31G level) on Gaussian 09 software.



Figure S2. Normalized UV-vis absorption (solid line) and fluorescence emission (dash line) spectra of 2B and 3B in toluene (a), THF (b) and DMF (c) $(5.0 \times 10^{-6} \text{ M}, \lambda_{ex} = 400 \text{ nm}).$



Figure S3. Fluorescence emission spectra of **2B** excited at 350 nm in as-prepared crystal (navy); ground powder (black); ground powder was heated at 100 °C for 1 min (red), at 100 °C for 30 min (blue) and at 200 °C for 10 min (magenta).



Figure S4. UV-vis absorption spectra of 2B (a) and 3B (b) in different solid states.



Figure S5. XRD patterns of compound 3B in as-prepared crystal, ground powder, and fumed sample.



Figure S6. DSC thermograms of 2B (a) and 3B (b) in as-prepared crystal (solid line) and ground powder (dash line) under nitrogen atmosphere at a heating rate of 10 °C \min^{-1} .



Figure S7 ¹H NMR (400 MHz, CDCl₃) spectrum of 1B.



Figure S8¹³C NMR (100 MHz, CDCl₃) spectrum of 1B.







Figure S10 ¹H NMR (400 MHz, CDCl₃) spectrum of 2B.







Figure S12 MALDI/TOF MS spectrum of 2B.



Figure S13 ¹H NMR (400 MHz, CDCl₃) spectrum of 3B.



Figure S14¹³C NMR (100 MHz, CDCl₃) spectrum of 3B.



Figure S15 MALDI/TOF MS spectrum of 3B.