Fluorescent Mesogenic Boron Difluoride Complexes Derived from Heterocyclic Benzoxazoles

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1. Single Crystal Data

Table S1. Bond lengths [Å] and angles [°] crystal **1a** (m = 12, n = 8).

Crystal **1a** (n = 8)			
Bond distances			
B(1)-F(1)	1.379(4)	B(1)-F(2)	1.385(5)
B(1)-O(2)	1.443(5)	B(1)-N(1)	1.571(4)
B(2)-F(3)	1.374(4)	B(2)-F(4)	1.382(5)
B(2)-O(6)	1.448(5)	B(2)-N(2)	1.575(4)
Bond angles			
F(1)-B(1)-F(2)	110.8(4)	F(1)-B(1)-O(2)	110.4(3)
F(2)-B(1)-O(2)	111.2(3)	F(1)-B(1)-N(1)	109.3(3)
F(2)-B(1)-N(1)	107.1(3)	O(2)-B(1)-N(1)	108.0(3)
F(3)-B(2)-F(4)	111.3(3)	F(3)-B(2)-O(6)	110.4(3)
F(4)-B(2)-O(6)	111.5(3)	F(3)-B(2)-N(2)	108.8(3)
F(4)-B(2)-N(2)	106.8(3)	O(6)-B(2)-N(2)	107.9(3)

2. Layered structure proposed in crystalline phase

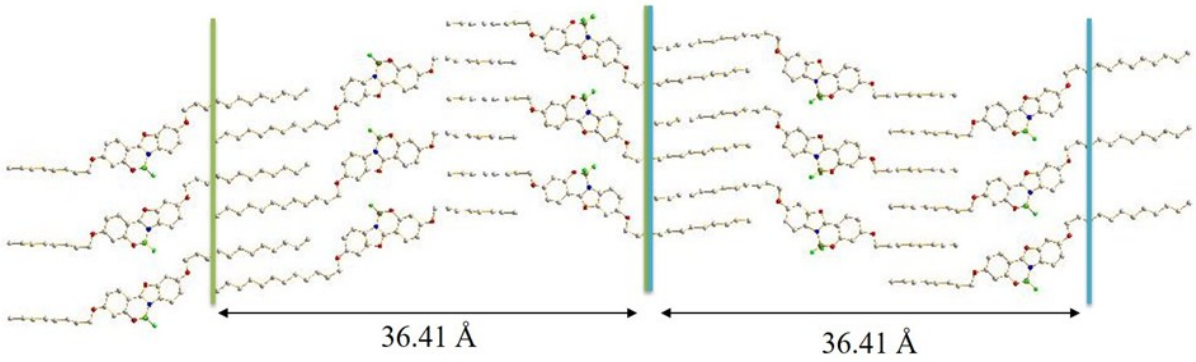

Fig. S1 Layered structures formed in crystal lattice by crystal **1a** (n = 8). Solid line represents the neighboring layers in the crystal lattice. The distance between layers is 36.41 Å in **1a**.

3. X–Ray Diffraction Plot

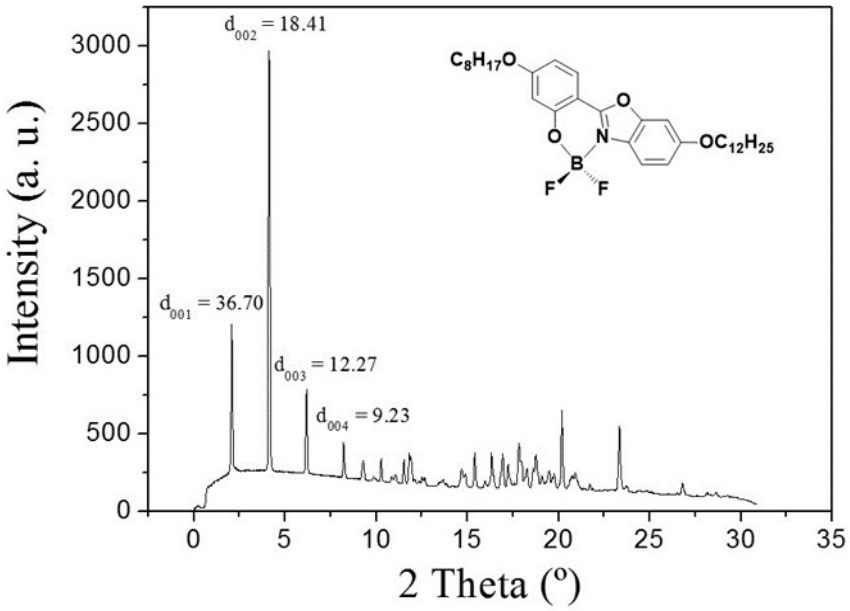

Fig. S2 The powder X–ray diffraction plot of compound **1a** (n = 8) at 25 °C.

4. The ^{1}H and ^{13}C NMR spectra of compounds 2a and 1a

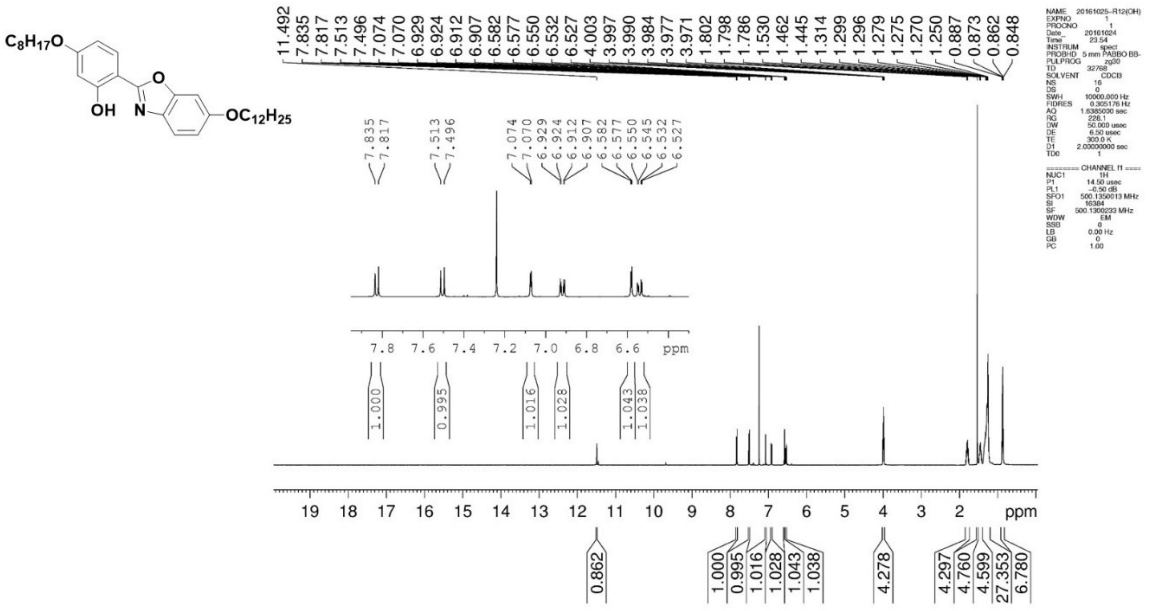

Fig. **S3** The ^{1}H-NMR spectrum of compound **2a** (n = 8).

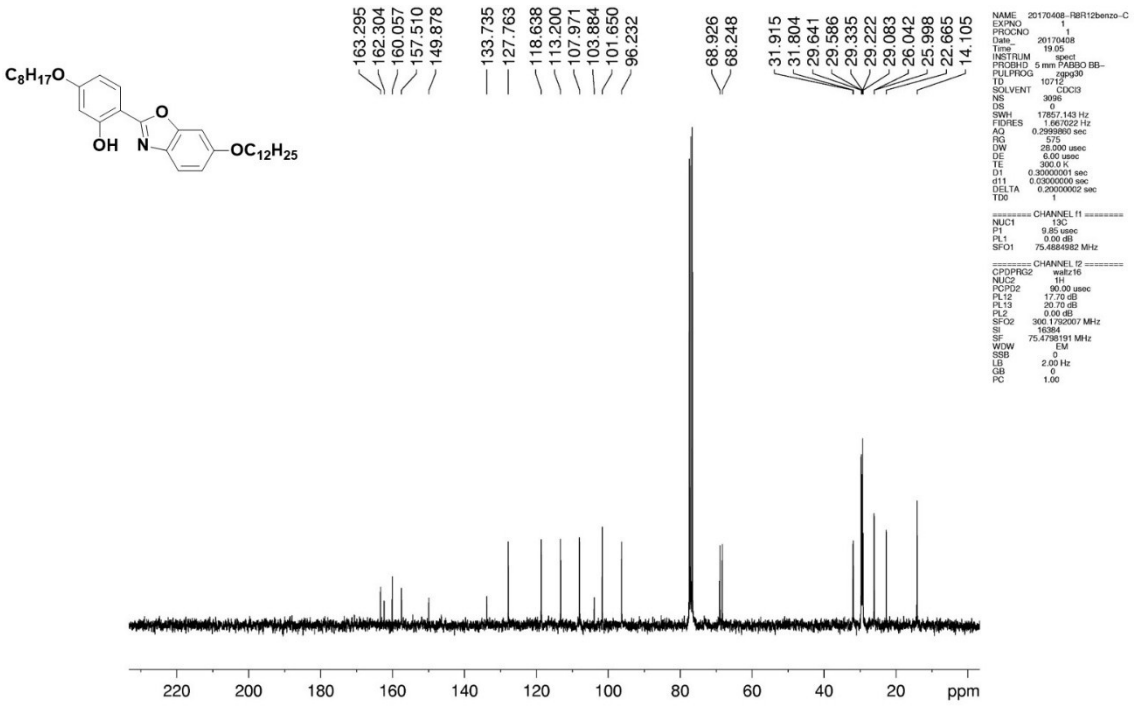

Fig. **S4** The [13]C-NMR spectrum of compound **2a** (n = 8).

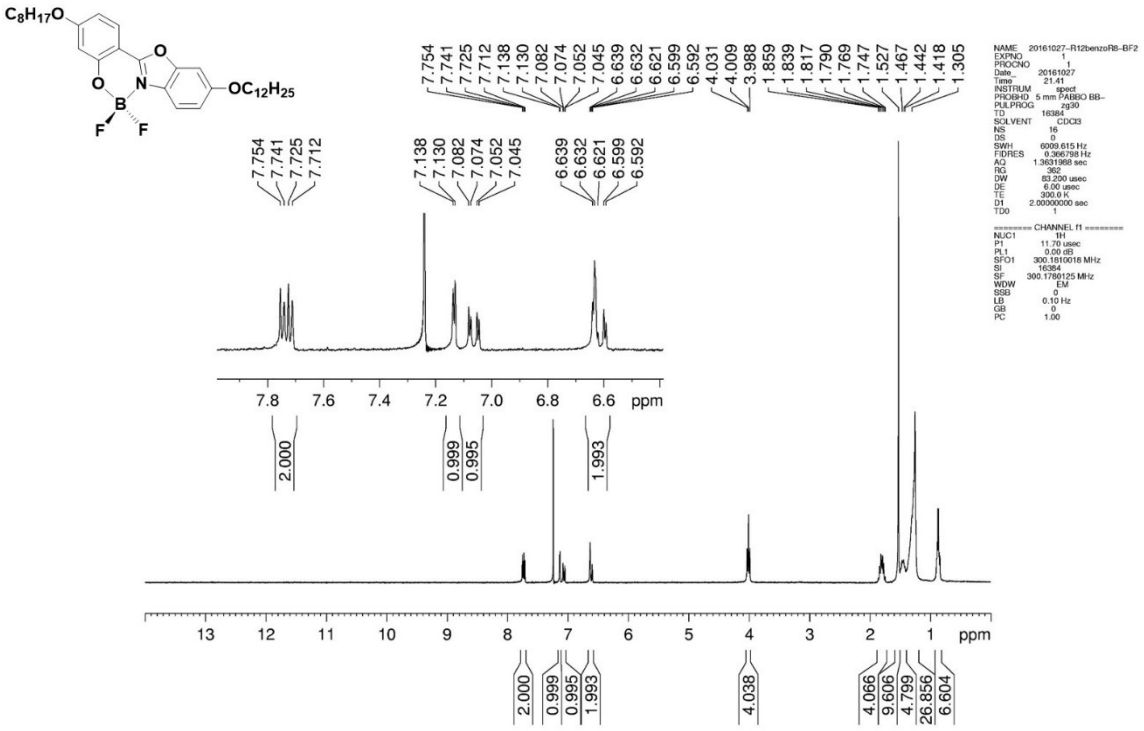

Fig. **S5** The [1]H-NMR spectrum of compound **1a** (n = 8).

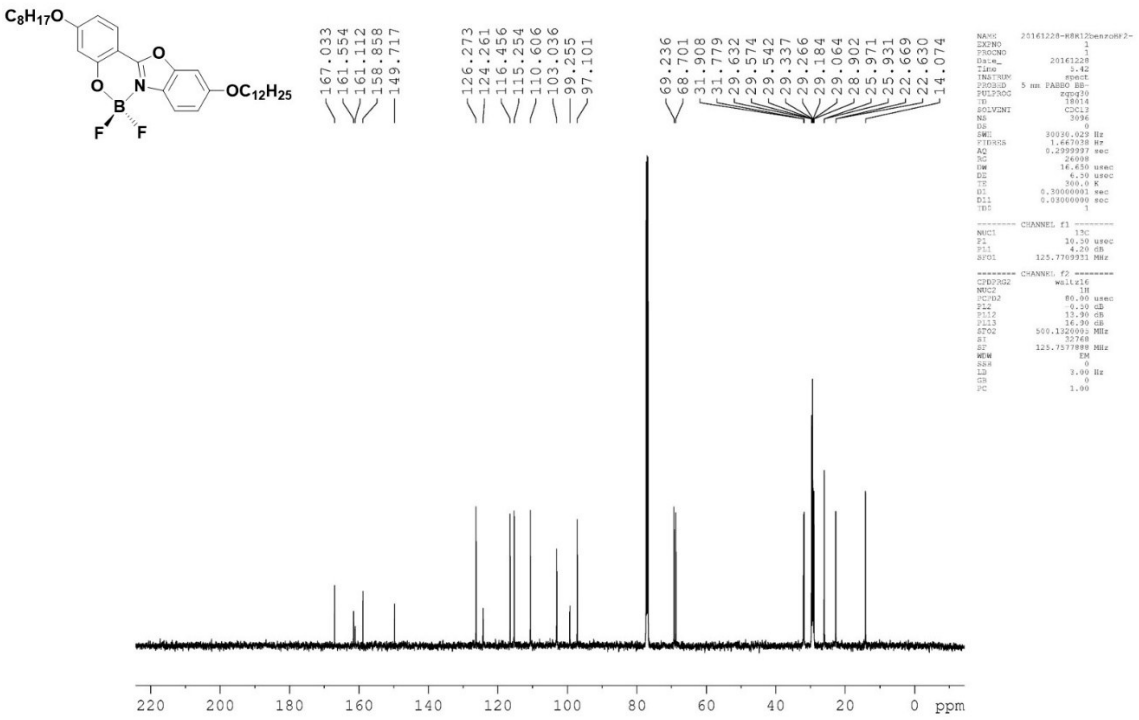

Fig. **S6** The ^{13}C-NMR spectrum of compound **1a** (n = 8).

4. The DSC Thermographs of Compounds 2a and 1a

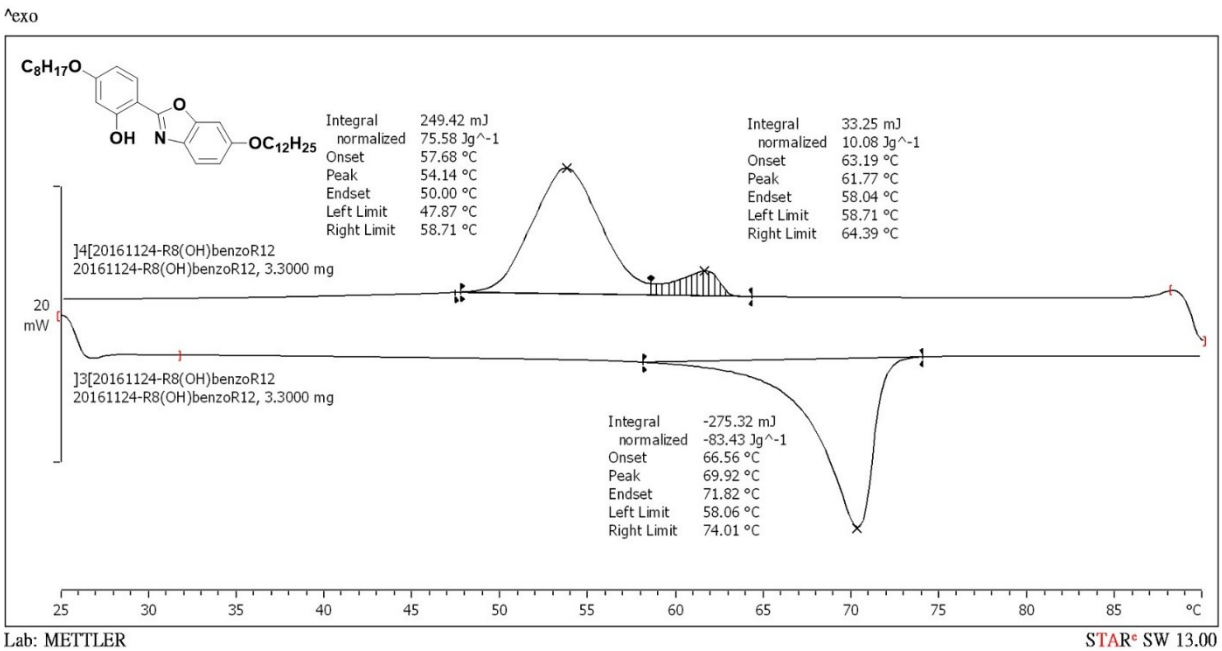

Fig. **S7** DSC thermograph of compound **2a** (n = 8).

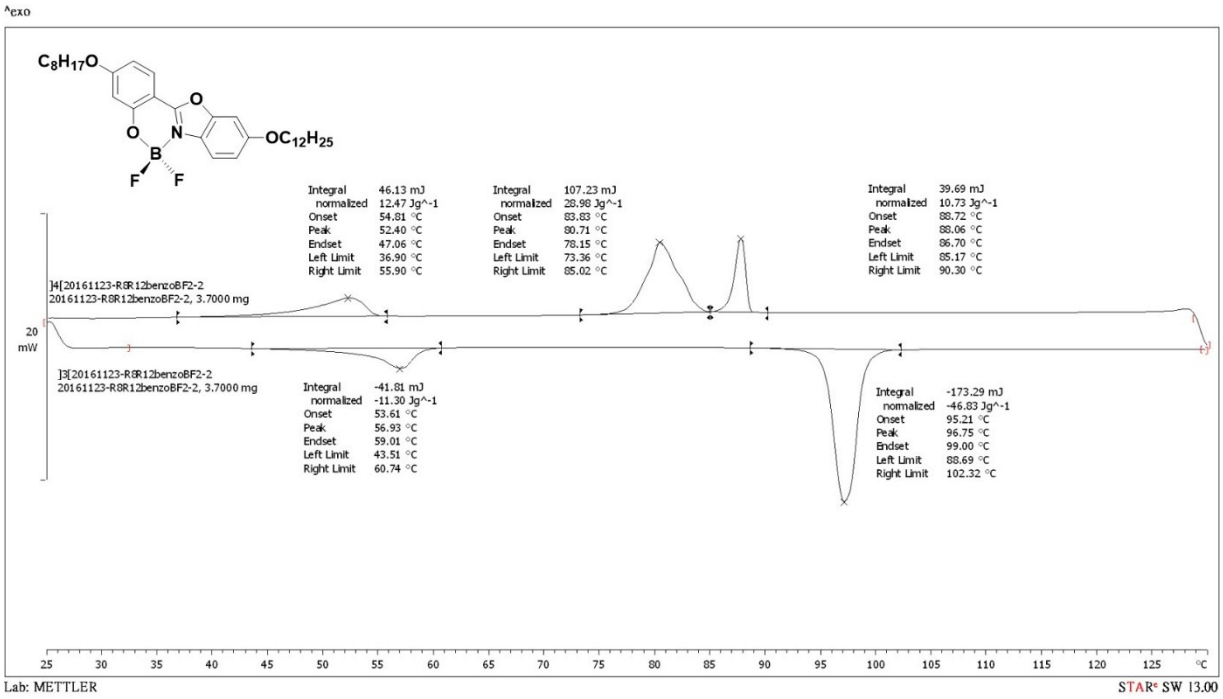

Fig. **S8** DSC thermograph of compound **1a** (n = 8).

6. Optical Property

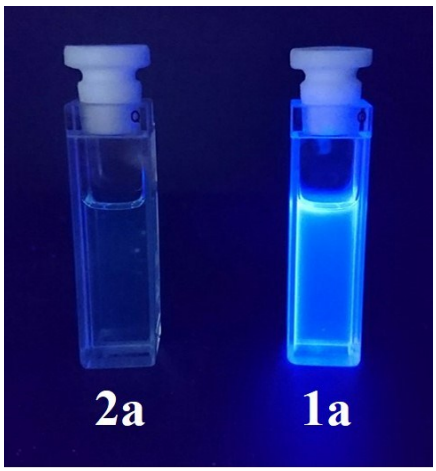

Fig. S9 Fluorescence emitted by compounds **1a** and **2a** in dichloromethane (~10^{-5} M) under exposed long wavelength UV light.