Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Solid-state Emissive Triarylborane-based BODIPY Dyes: Photophysical Properties and Fluorescent Sensing for Fluoride and Cyanide Ions

Guang-Liang Fu, Hong Pan, Yi-Hong Zhao and Cui-Hua Zhao*

School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China,

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Titration Measurement

Titration of 1 with TBAF

All the fluorescence experiments were recorded in a THF solution of **1** (c = 4.28× 10^{-6} M). The solution of **1** (2 ml in a quartz cuvette) was titrated with incremental amounts of fluoride by addition of a concentrated TBAF solution (c = 4.56 × 10^{-4} M). In order to account for dilute effects, the TBAF solution also contained **1** at its initial concentration.

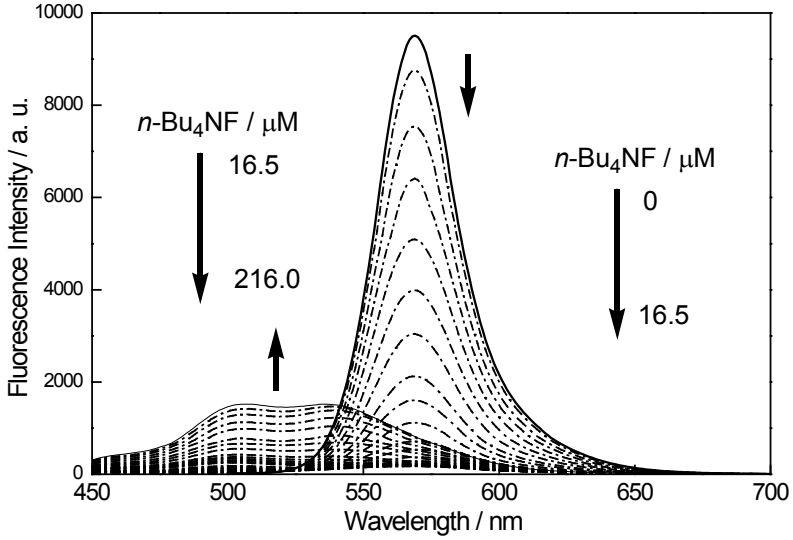


Figure S-1 The fluorescence spectra change of **1** (4.28 μM in THF) upon addition of TBAF.

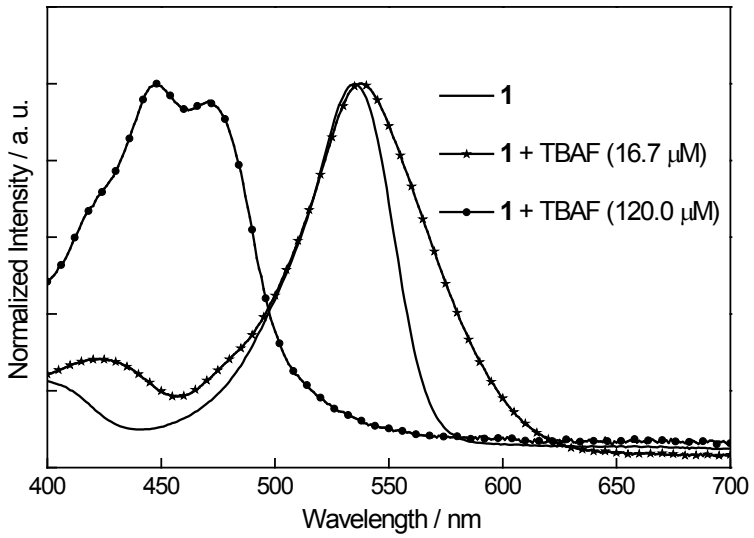


Figure S-2 The UV/vis absorption spectra change of **1** (4.28 μM in THF) upon addition of TBAF.

Titration of 2 with TBAF

All the fluorescence experiments were recorded in a THF solution of **2** (c = 2.61 × 10^{-6} M). The solution of **2** (2 ml in a quartz cuvette) was titrated with incremental amounts of fluoride by addition of a concentrated TBAF solution (c = 4.63 × 10^{-4} M). In order to account for dilute effects, the TBAF solution also contained **2** at its initial concentration.

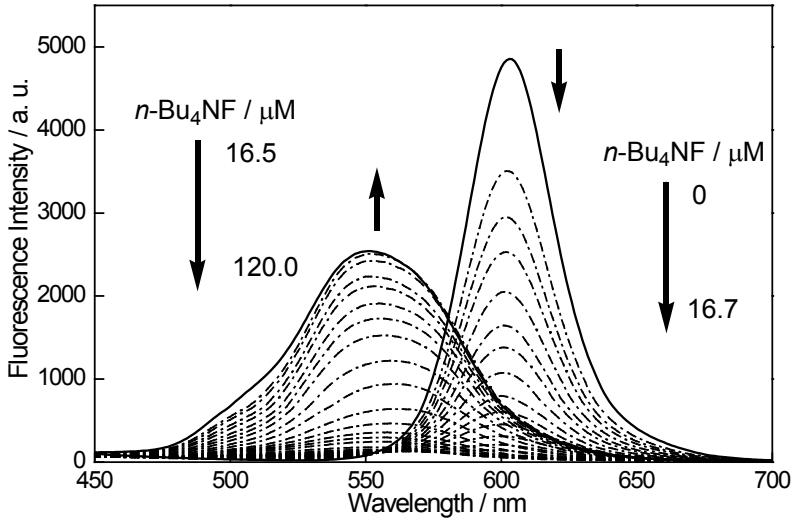


Figure S-3 The fluorescence spectra change of **2** (2.61 μM in THF) upon addition of TBAF.

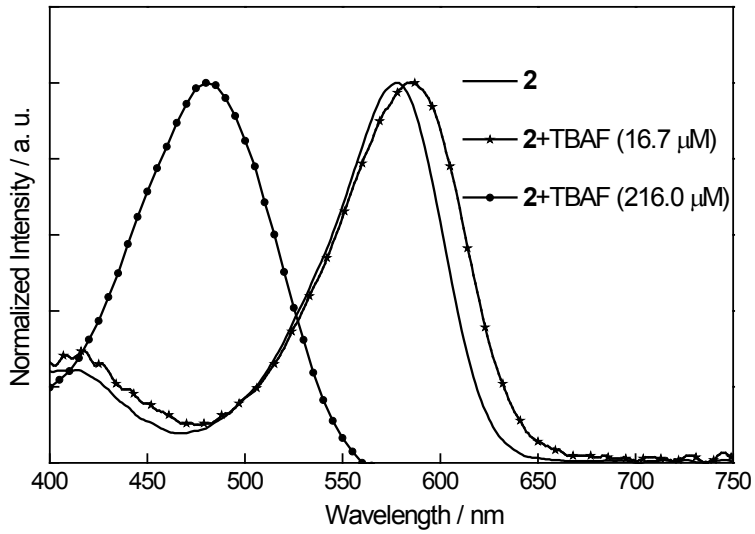


Figure S-4. The UV/vis absorption spectra change of **2** (2.61 μM in THF) upon addition of TBAF.

^{11}B NMR Measurement of 1

The ^{11}B NMR spectra of a solution of **1** (0.5 mL, 0.03 M, $CDCl_3$) were obtained before and after the addition of an excess of fluorid.

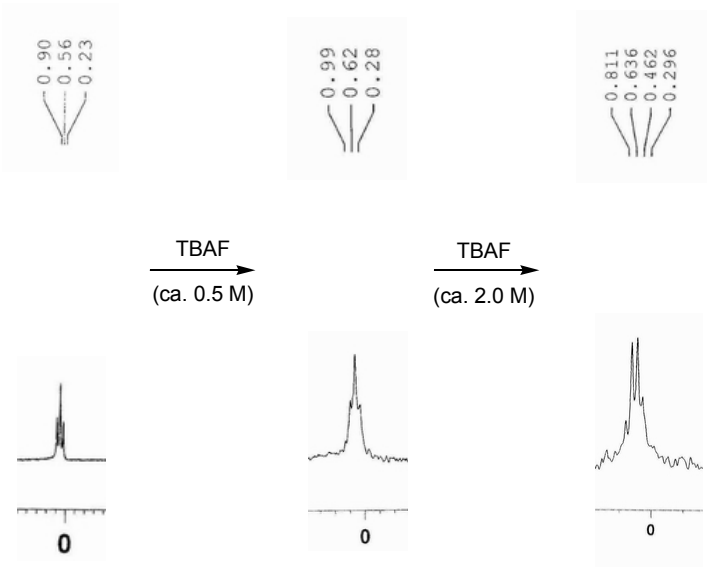


Figure S-5. ^{11}B NMR spectra of **1** (0.03M in $CDCl_3$) upon addition of TBAF.

^{11}B NMR Measurement of 2

The ^{11}B NMR spectra of a solution of **2** (0.5 mL, 0.03 M, $CDCl_3$) were obtained before and after the addition of an excess of fluoride.

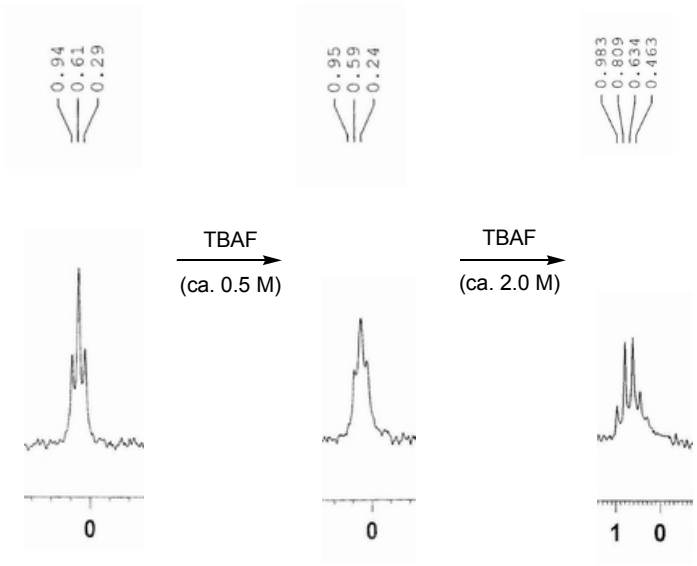


Figure S-6. ^{11}B NMR spectra of **2** (0.03M in $CDCl_3$) upon addition of TBAF.

Titration of 1 with TBACN

All the fluorescence experiments were recorded in a THF solution of **1** (c = 4.28× 10^{-6} M). The solution of **1** (2 ml in a quartz cuvette) was titrated with incremental amounts of cyanide by addition of a concentrated TBACN solution (c = 4.28 × 10^{-4} M). In order to account for dilute effects, the TBACN solution also contained **1** at its initial concentration.

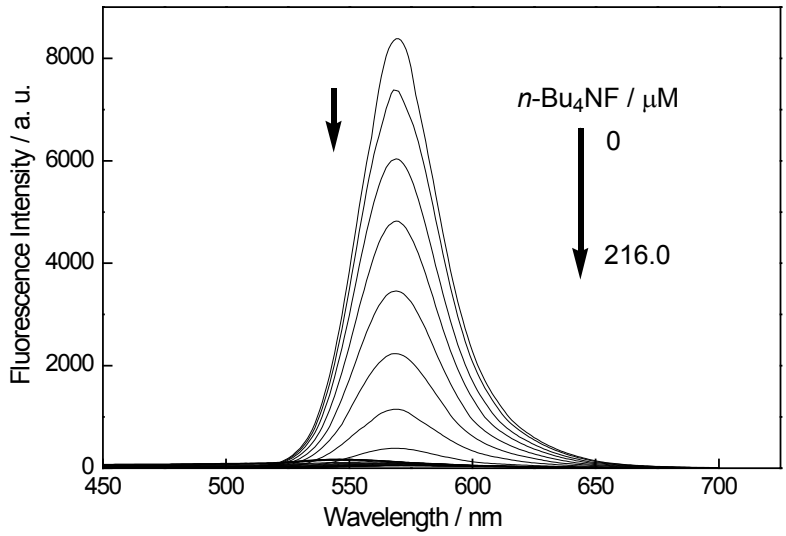


Figure S-7. Fluorescence spectra change of (a) **1** (4.28 μM in THF, λ_{ex} = 370 nm) upon addition of TBACN.

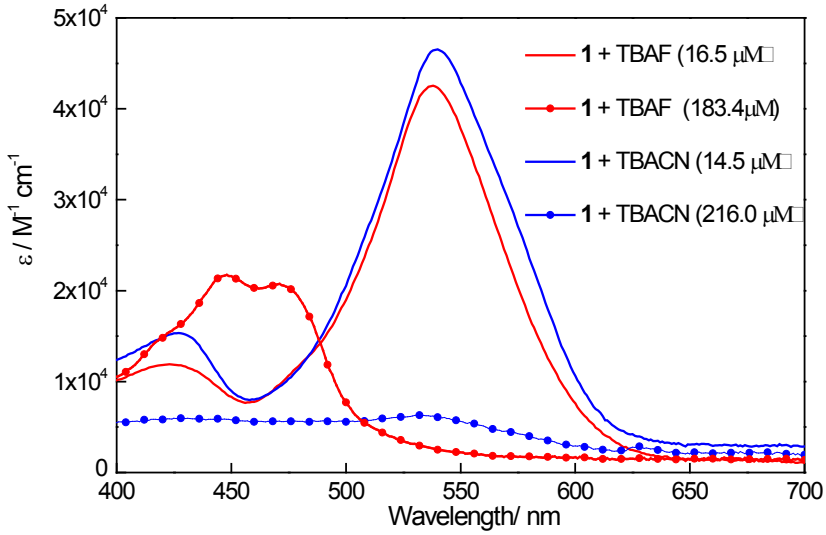


Figure S-8. The UV/vis absorption spectra of **1** in THF (4.28 μM) after addition of excess TBAF and TBACN.

Titration of 2 with TBACN

All the fluorescence experiments were recorded in a THF solution of **1** (c = 2.61× 10^{-6} M). The solution of **2** (2 ml in a quartz cuvette) was titrated with incremental amounts of cyanide by addition of a concentrated TBACN solution (c = 5.21 × 10^{-4} M). In order to account for dilute effects, the TBACN solution also contained **2** at its initial concentration.

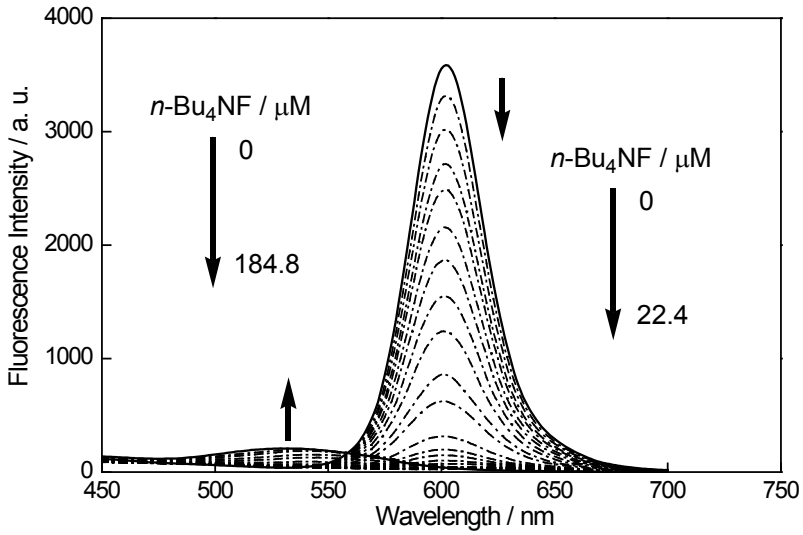


Figure S-9. Fluorescence spectra change of (a) **2** (2.61 μM in THF, λ_{ex} = 370 nm) upon addition of TBACN.

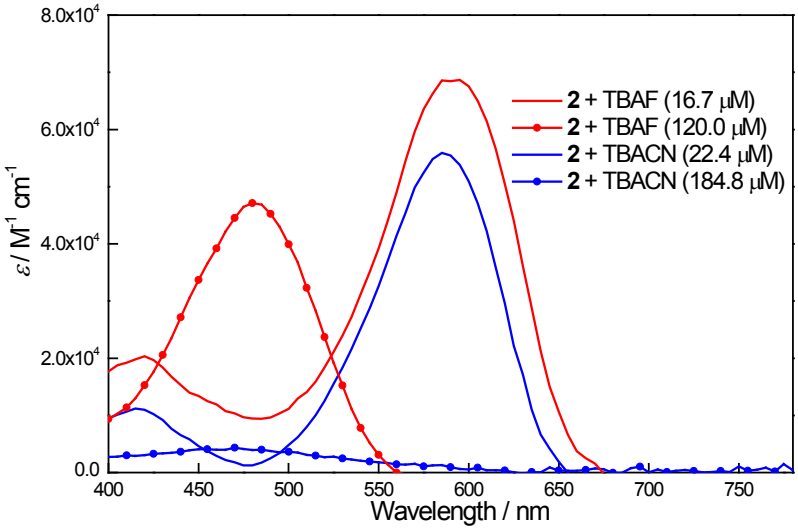
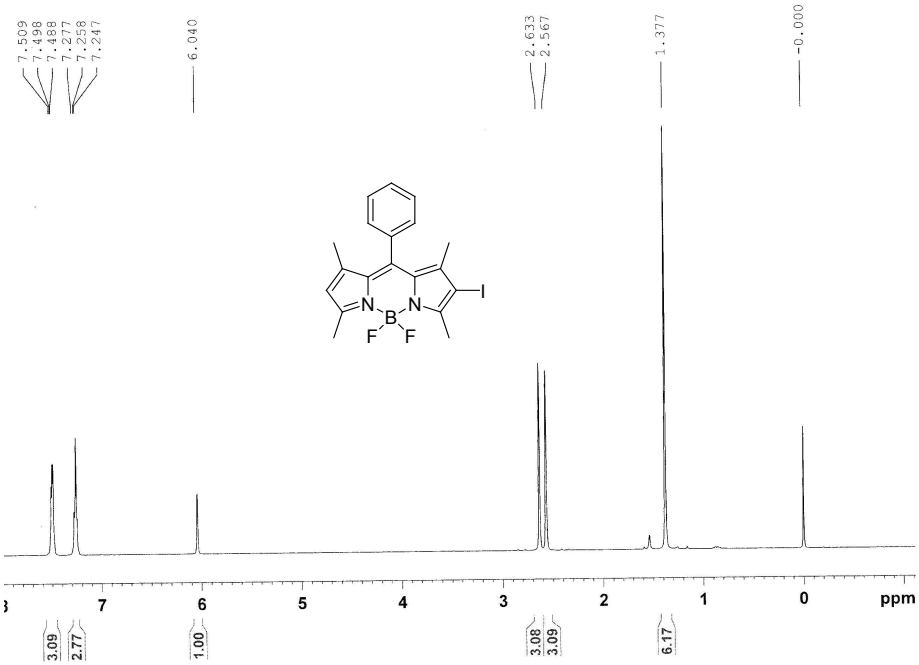


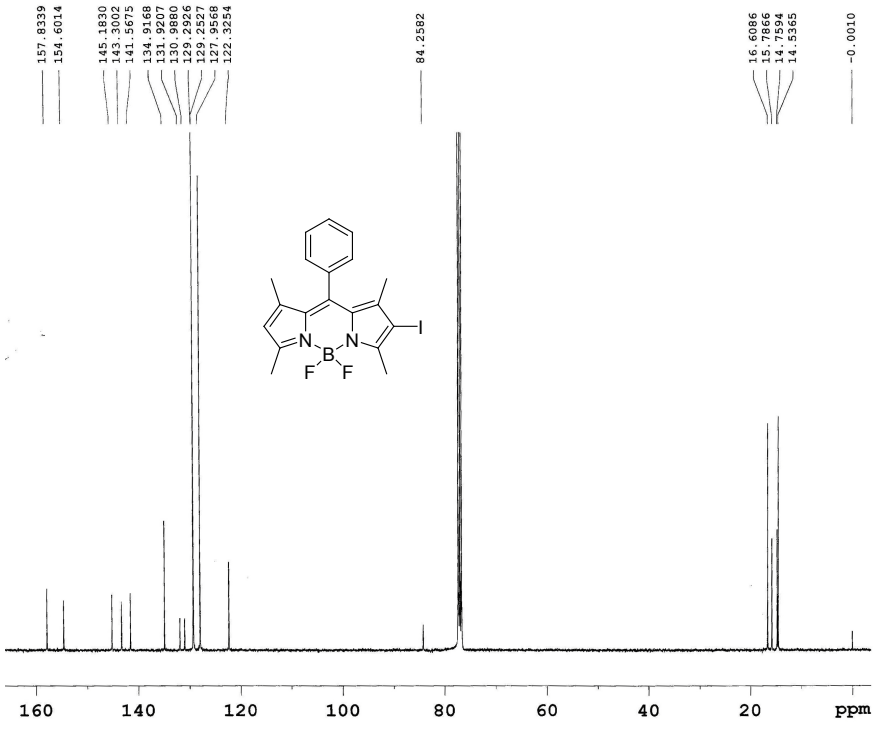
Figure S-10. The UV/vis absorption spectra of **2** in THF (2.61 μM) after addition of excess TBAF and TBACN.

NMR Spectra

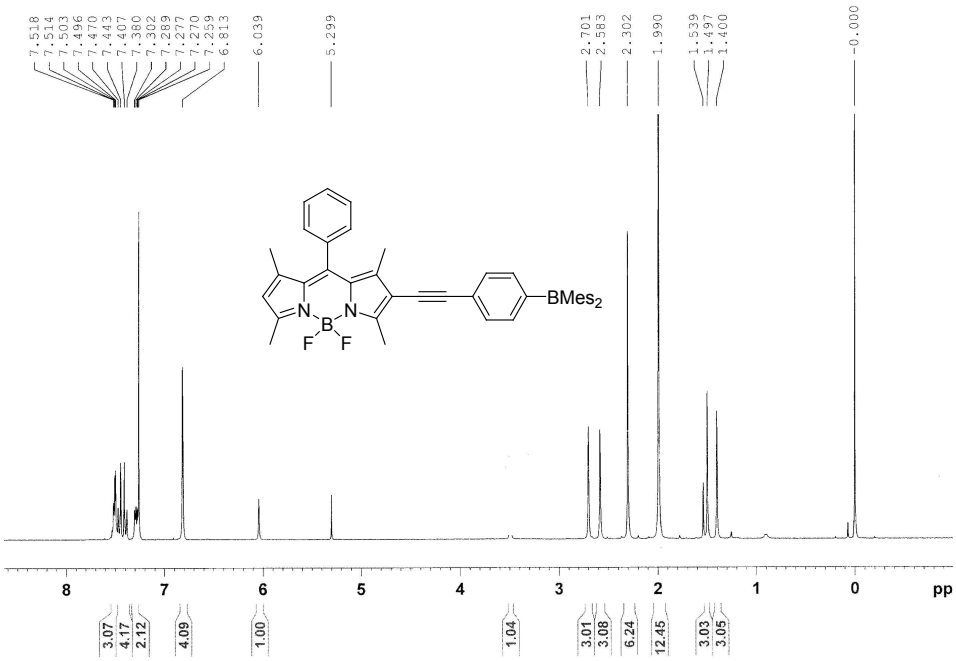
^{1}H NMR of **4** (300 MHz, $CDCl_3$)



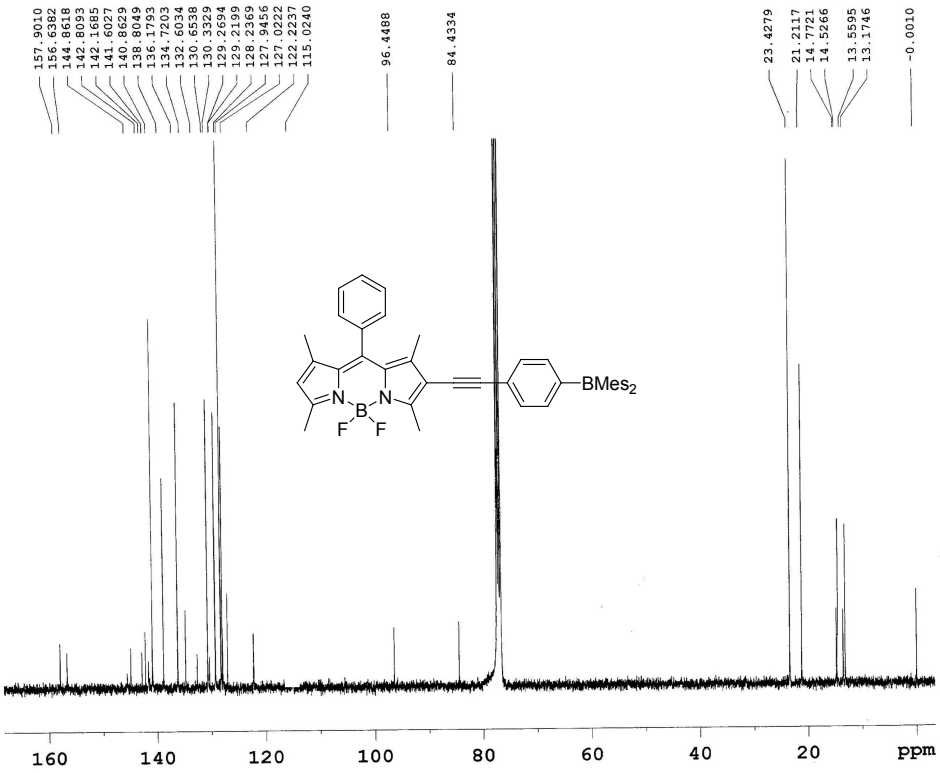
^{13}C NMR of **4** (400 MHz, $CDCl_3$)



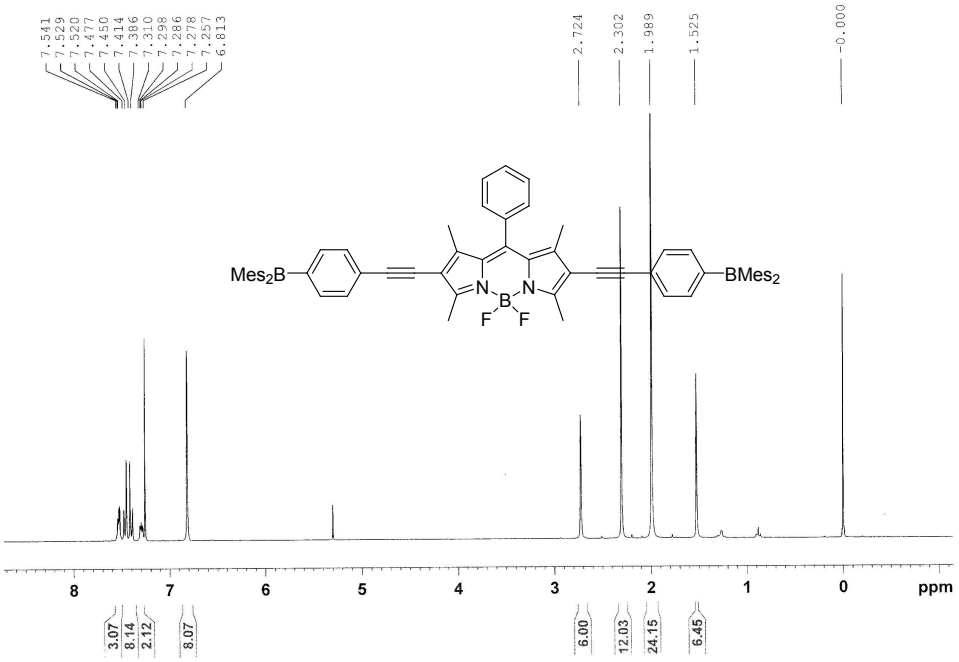
^{1}H NMR of **1** (300 MHz, $CDCl_3$)



^{13}C NMR of **1** (400 MHz, $CDCl_3$)



^{1}H NMR of **2** (300 MHz, $CDCl_3$)



^{13}C NMR of **2** (400 MHz, $CDCl_3$)