Supporting Information

Synthesis, Structure, Spectral, Electrochemical and Fluoride Sensing Properties of *meso*-Pyrrolyl Boron Dipyrrromethene
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Calcd mol. wt. = 280.0830
Observed mol. Wt. = 280.0826
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Calcd mol. wt. = 357.9936
Observd mol. Wt. = 357.9920
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Figure S31: Comparison of absorption spectra of compound 7 (2×10^{-5}M) recorded in different solvents.
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Figure S38. Job’s plots of compound 5
Figure 39. Supramolecular assembly through a weak intermolecular hydrogen bonding network in BODIPY 5.
Figure 40. Supramolecular assembly through intermolecular-hydrogen bonding network (between Methyl-H and F (2.247 Å) which is attached to boron in Compound 6.
Figure 41. Optical response of BODIPY 5 after addition of different anions
Experimental section

General: THF and n-hexane was dried over sodium benzophenone ketyl, BF$_3$, Et$_2$O, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and TFA were used as obtained. All other chemicals used for the synthesis were reagent grade unless otherwise specified. Column chromatography was performed on silica (60-120 mesh) or alumina. All the $^1$H NMR spectra ($\delta$ in ppm) were recorded using Bruker 400 and 500 MHz instruments. $^{13}$C NMR spectra were recorded on Bruker operating at 100.6 and 125.7 MHz. TMS was used as an internal reference for $^1$H and $^{13}$C ($\delta$ 77.0 signal) in CDCl$_3$. For UV-vis, the stock solution of compound 5 ($2\times10^{-5}$ M) was prepared by using spectroscopic grade toluene.

Their corresponding UV-vis was recorded at 298 K. In $^1$H NMR titration, the spectra were measured on 400 MHz NMR spectrometer. A solution of 5 in CDCl$_3$ was prepared ($2\times10^{-5}$ M), and a 0.4 mL portion of this solution was transferred to a 5-mm NMR tube. A small aliquot of Bu$_4$NF in CDCl$_3$ was added in an incremental fashion, and their corresponding spectra were recorded.
X-ray crystal structure analysis:

Single-crystal X-ray structure analysis was performed on a Rigaku Saturn 724 diffractometer that was equipped with a low-temperature attachment. Data were collected at 100 K using graphite-monochromated Mo-K\(_\alpha\) radiation (\(\lambda_{\alpha} = 0.71073\ \text{Å}\)) with the \(\omega\)-scan technique. The data were reduced by using CrystalClear-SM Expert 2.1 b24 software. The structures were solved by direct methods and refined by least-squares against \(F^2\) utilizing the software packages SHELXL-97,\(^{33}\) SIR-92,\(^{34}\) and WINGX.\(^{35}\) All non-hydrogen atoms were refined anisotropically.

References:


Figure 42. Absorption spectra of compound 5 (2×10⁻⁵M) and after addition of HPO₄²⁻, H₂PO₄⁻ recorded in Toluene
Figure 43. Absorption spectral change of compound 5 (2×10⁻⁵M) and after addition of different equivalents of F⁻ (0-50 equiv.) recorded in CH₃OH.
Figure 44. Absorption spectral changes of BODIPY 5 (2×10^{-5} M) upon addition of increasing equivalents of F^{-} ions (0–15 equiv) in CH_{3}CN.
**Figure 45.** Absorption spectral changes of BODIPY 5 (2×10⁻⁵ M) upon addition of increasing equivalents of F⁻ ions (0–50 equiv) in CH₃CN:H₂O (9:1).