Charge Transfer Emission Involving Three-Coordinate Organoboron: V-Shape versus U-Shape and Impact of the Spacer on Dual Emission and Fluorescent Sensing

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HOMO-LUMO diagrams of 2

2nd LUMO (1.47 eV)  LUMO (1.92 eV)

2nd HOMO (6.17 eV)  HOMO (5.23 eV)
HOMO-LUMO diagrams of 3

2\text{nd} LUMO (1.55 eV)

LUMO (1.61 eV)

2\text{nu} HOMO (5.10 eV)

HOMO (5.06 eV)
HOMO-LUMO diagrams of BN
UV-Vis spectra (all recorded in solution of $\sim 1.0 \times 10^{-5}$ M)
Absorption coefficient (M\(^{-1}\) cm\(^{-1}\))

- hexane
- toluene
- THF
- DCM
- DMF
- MeCN

Wavelength (nm)
The normalized emission spectra of BN in various solvents (BN is not soluble in CH₃CN and as a result the emission spectrum in CH₃CN was not recorded.)
The emission spectral change of sBN in DMF with time (2.01 x 10^{-5} M)
Correlation of Stokes shift of **SBNPB** versus \( E_{d}(30) \) polarity scale

\[
y = 216.22x - 3746.8 \quad R^2 = 0.9504
\]

Correlation of Stokes shift of **BNPB** versus \( E_{d}(30) \) polarity scale

\[
y = 305.1x - 6530 \quad R^2 = 0.9491
\]
The normalized emission spectra of 3 in various solvents.

![Normalized Emission Spectra](image)

The titration diagram of 3 in THF

![Titration Diagram](image)
The Plots of Stoke Shifts versus solvent polarity ($E_t(30)$ polarity scale) for the emission peak at the long wavelength of 1 and 3.

1

$y = 652.69x - 14690$

$R^2 = 0.9531$

3

$y = 636.24x - 13916$

$R^2 = 0.9723$
The Stern-Volmer plots of 3 after the addition of TBAF at the wavelengths of the two isosbestic points.
The ratiometric ($I_2/I_1$) Stern-Volmer plot of system C

![Ratiometric Stern-Volmer plot](image1.png)

NPB emission spectrum in DCM

![NPB emission spectrum](image2.png)
The emission spectral change of 3 after the addition of TBACl in THF
$^{19}$F NMR spectrum of 3 in the presence of excess TBAF in CH$_2$Cl$_2$. 

$^{19}$F NMR spectrum of BNPB in the presence of excess TBAF in CH$_2$Cl$_2$ before (top) and after (bottom) the addition of TBACl (TBAF:TBACl, 2:5).
The fluoride titration diagram of BN in CH₂Cl₂

The UV-Vis spectral change of sBN before and after the addition of F⁻ in CH₂Cl₂
UV-Vis of sBN in CH\textsubscript{2}Cl\textsubscript{2} before and after the addition of 40 eq. NBu\textsubscript{4}F
CV diagrams for 1 – 3 recorded in CH₂Cl₂ versus Ag/AgCl

![Graph of Compound 1](image1)

![Graph of Compound 2](image2)
CV diagrams for sBN (reduction, top; oxidation, bottom) in DMF versus Ag/AgCl