Electronic Supplementary Material (ESI) for New Journal of Chemistry

Tetraphenylethene-Decorated BODIPY Monomer/Dimer with Intense Fluorescence in Various Matrixes

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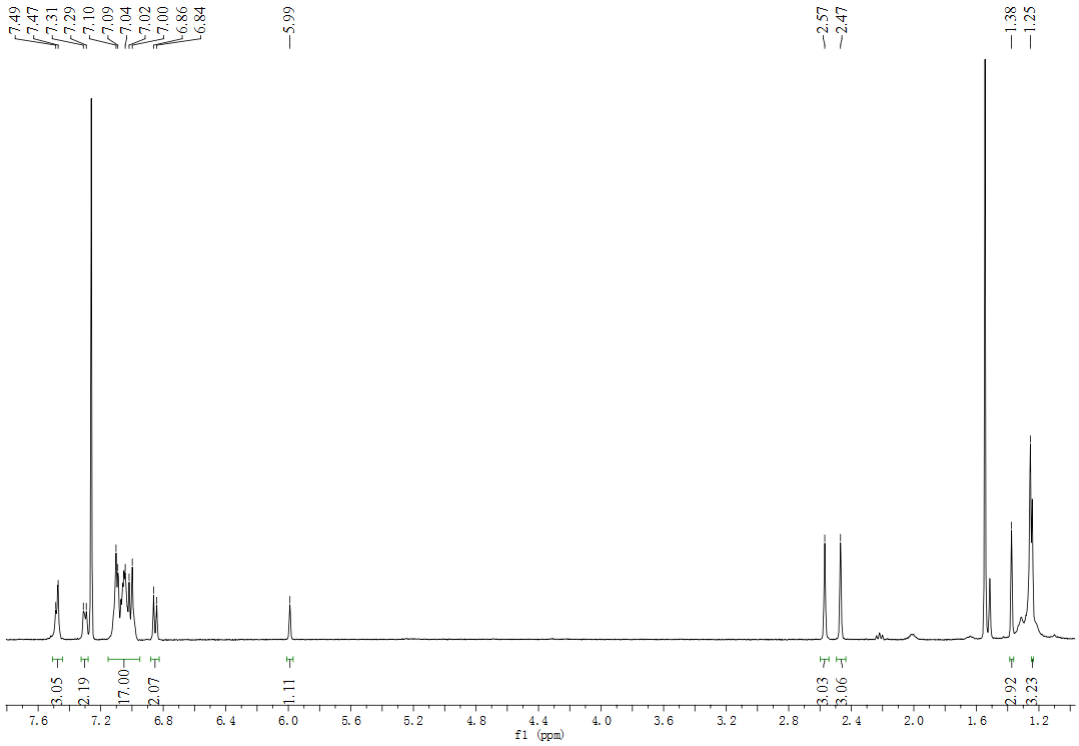
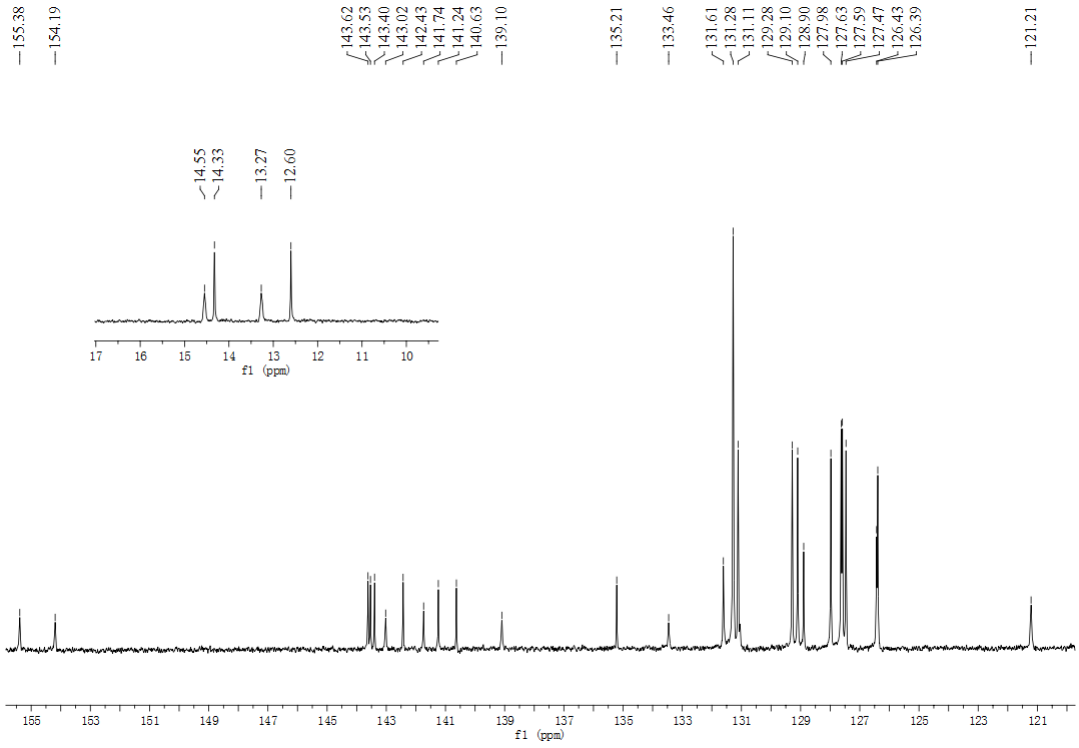
Supporting Information

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)

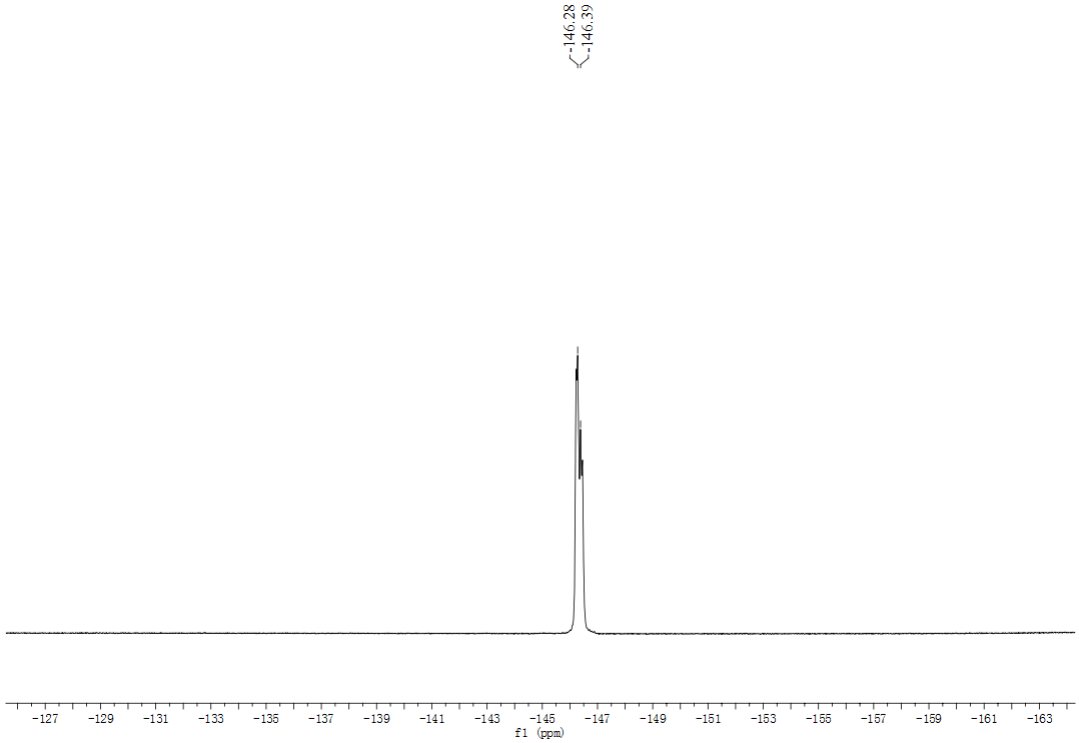
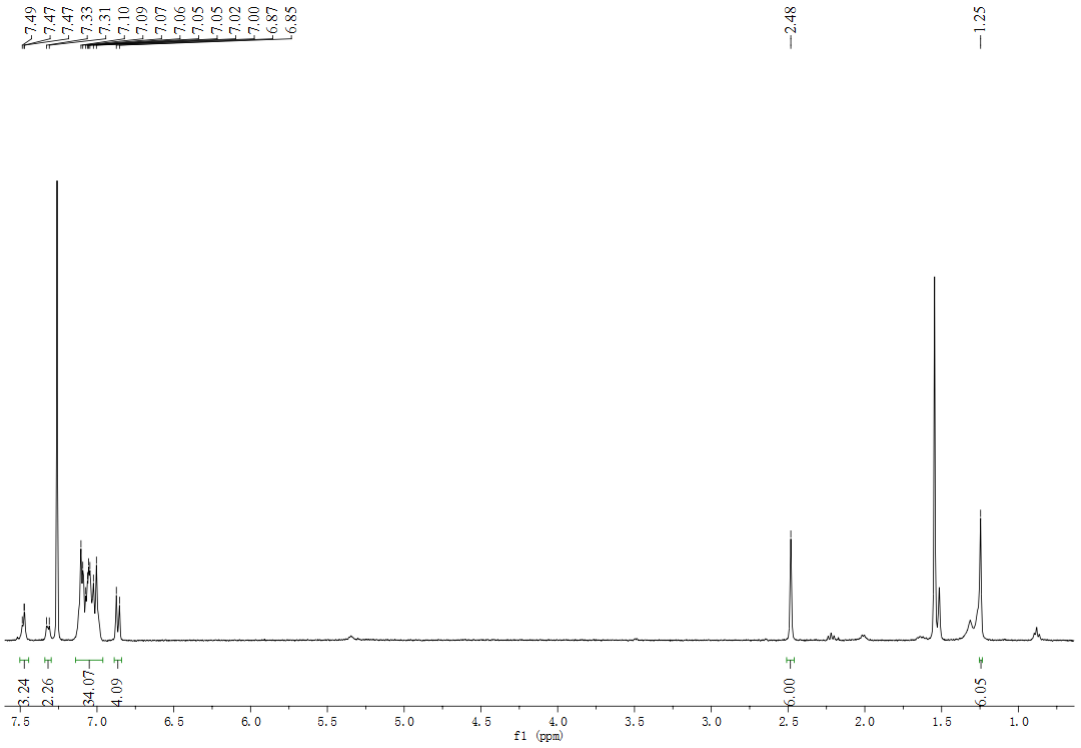
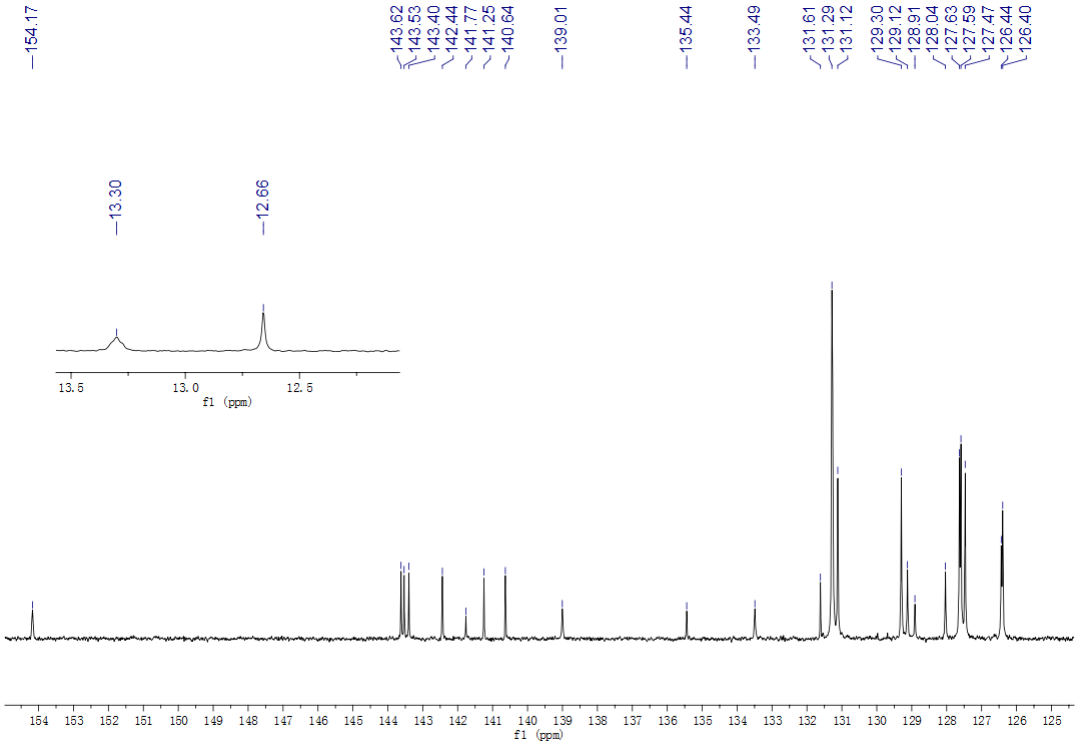


Figure S1. ^{1}H, ^{13}C and ^{19}F NMR spectra of **1** in $CDCl_3$.

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)

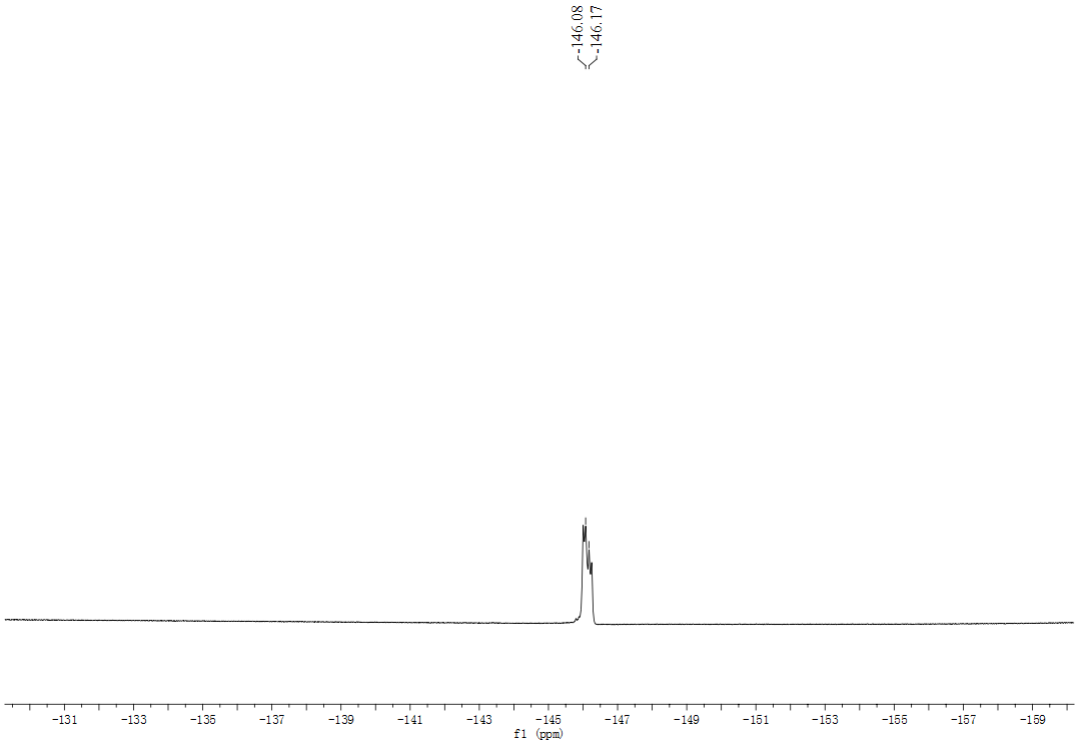
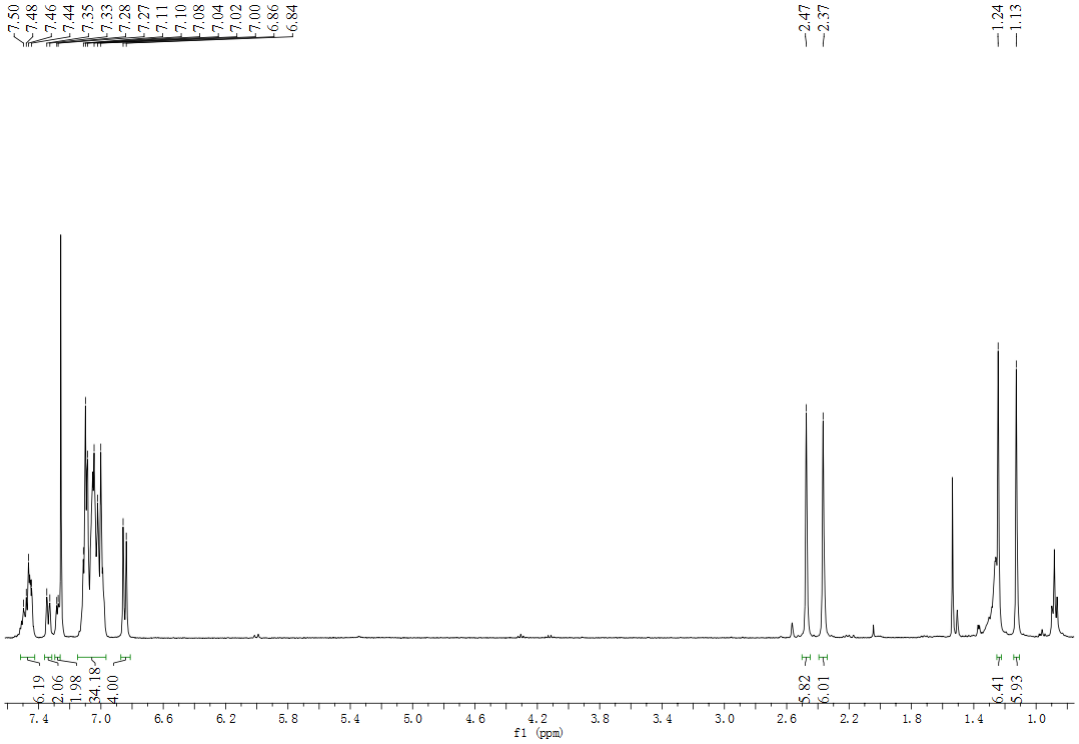
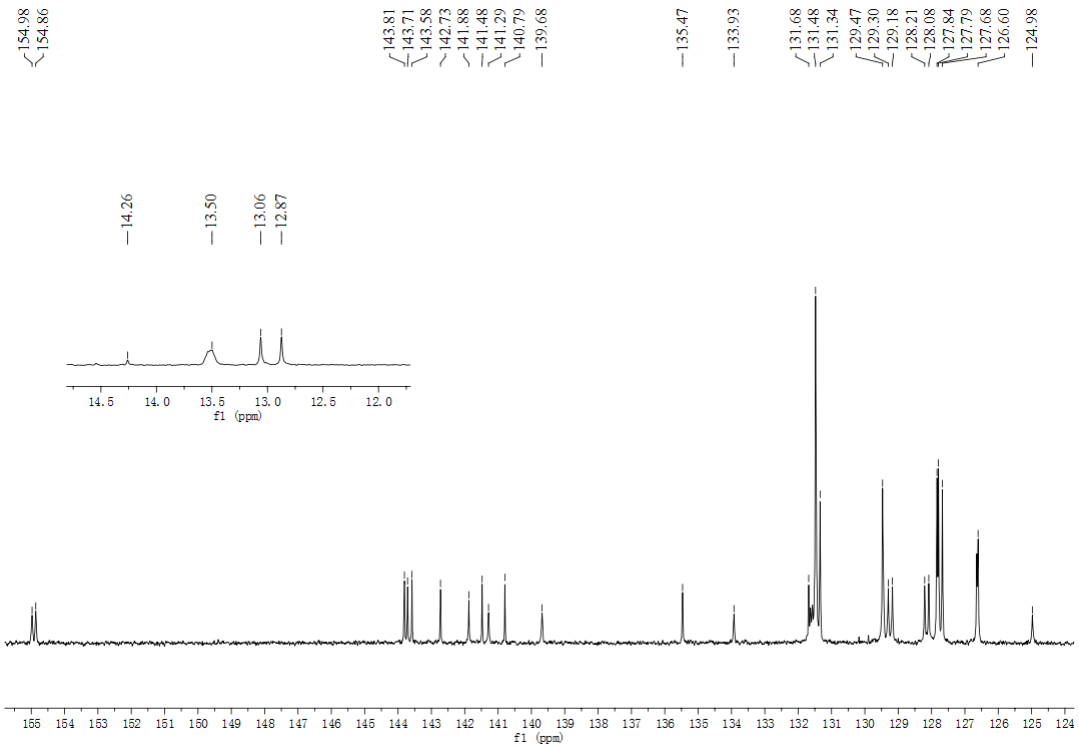


Figure S2. ^{1}H, ^{13}C and ^{19}F NMR spectra of **2** in $CDCl_3$.

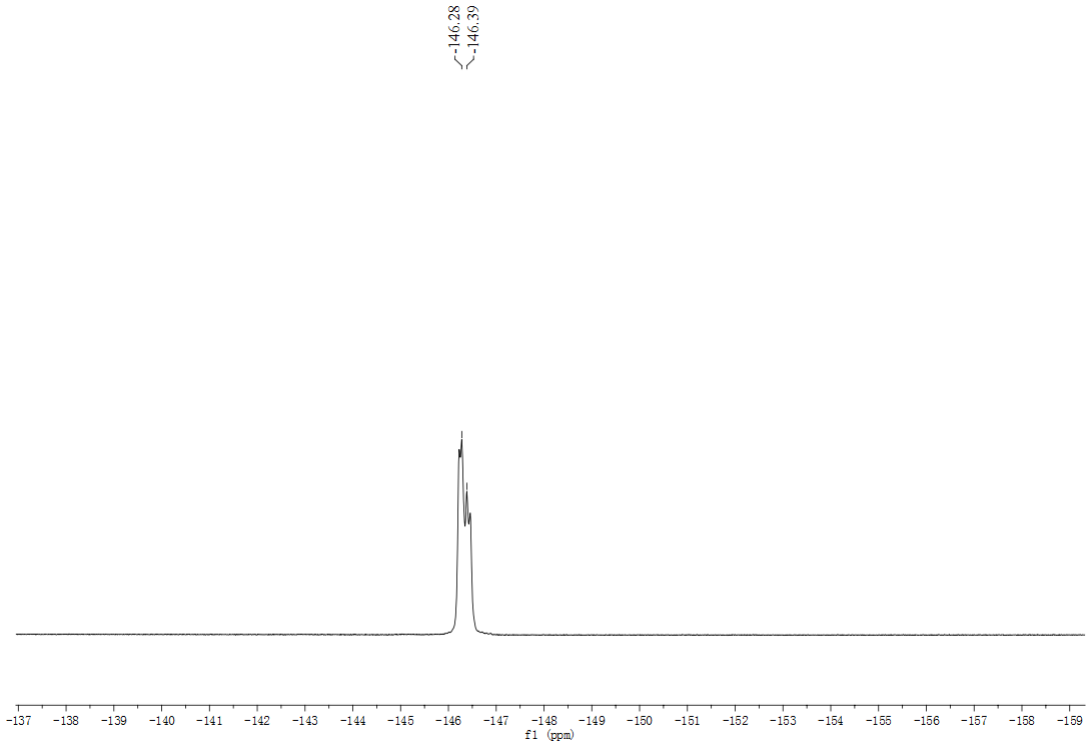
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)

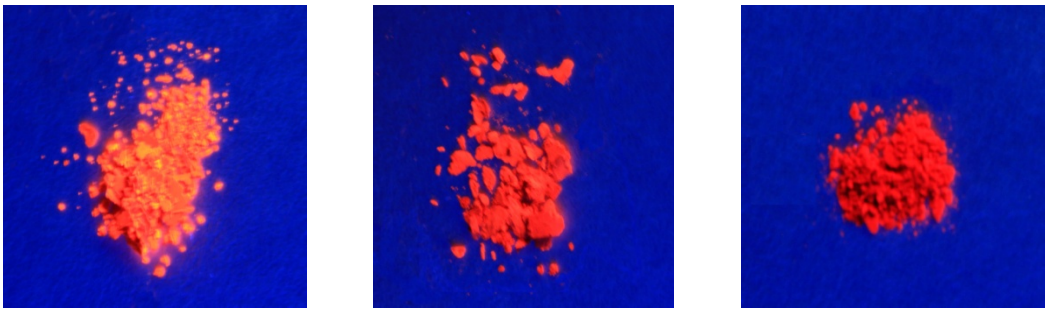


^{19}F NMR (376 MHz, $CDCl_3$)



(c)

Figure S3. ^{1}H, ^{13}C, ^{19}F NMR spectra of **3** in $CDCl_3$.



1 **2** **3**

Figure S4. Photographs of the powders **1**–**3** under the irradiation.

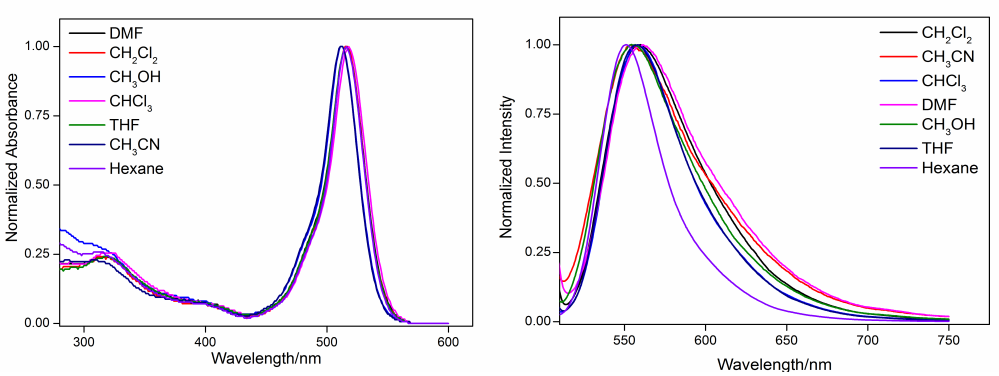


Figure S5. UV-Vis and fluorescence spectra of **1** in different solvents.

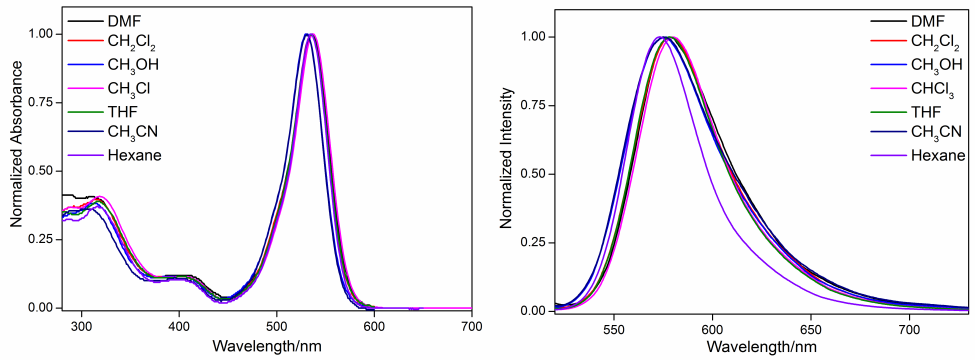


Figure S6. UV-Vis and fluorescence spectra of **2** in different solvents.

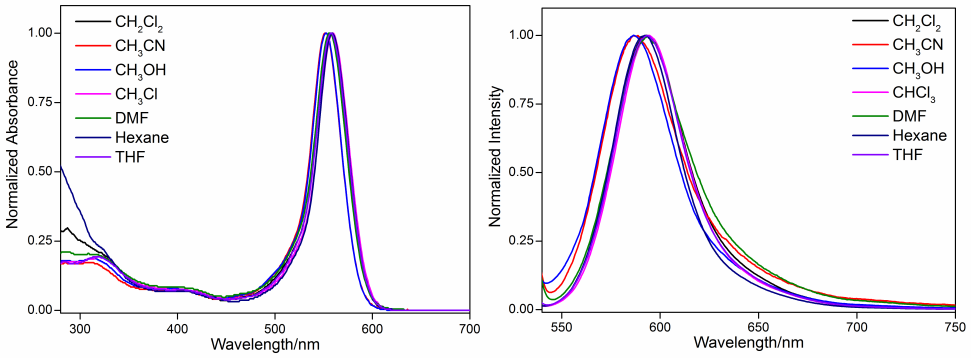


Figure S7. UV-Vis and fluorescence spectra of **3** in different solvents.

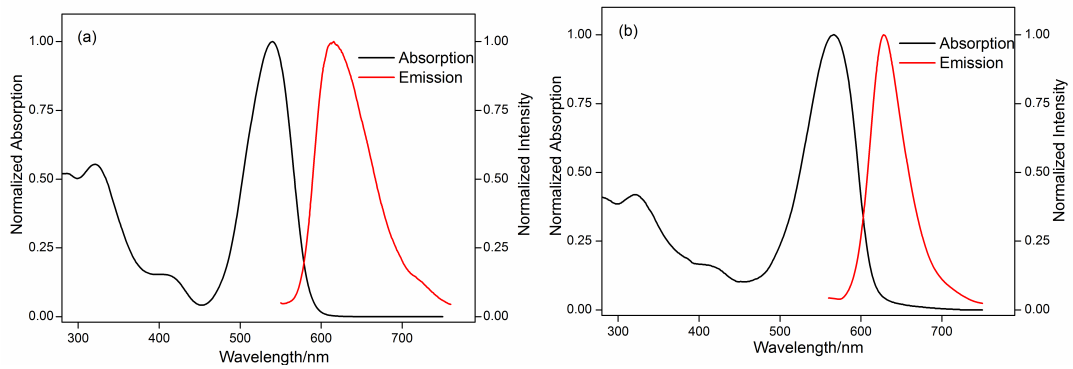


Figure S8.UV-Vis and fluorescence spectra of **2** (a) and **3** (b) in the solid state.

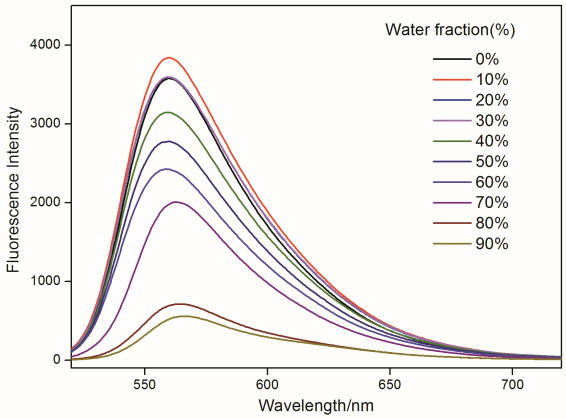


Figure S9 Fluorescence spectra of **1** in THF–H_2O mixture at different water fraction.

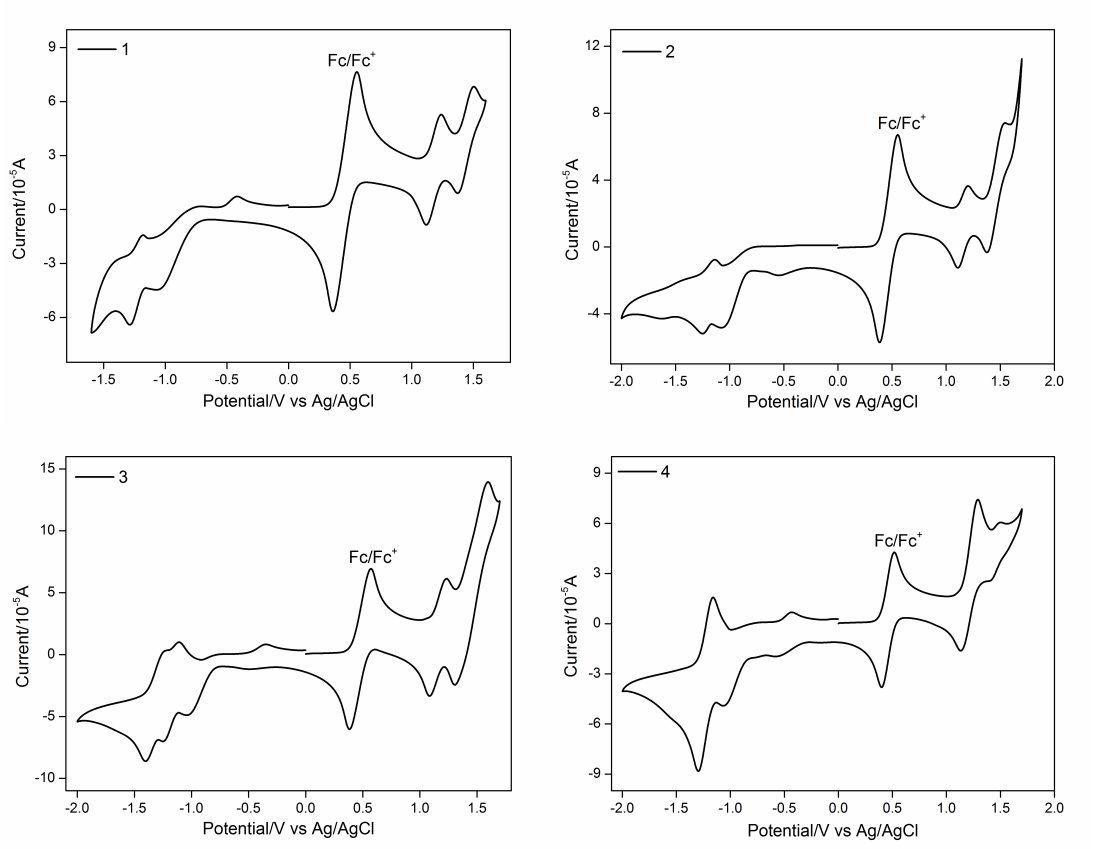
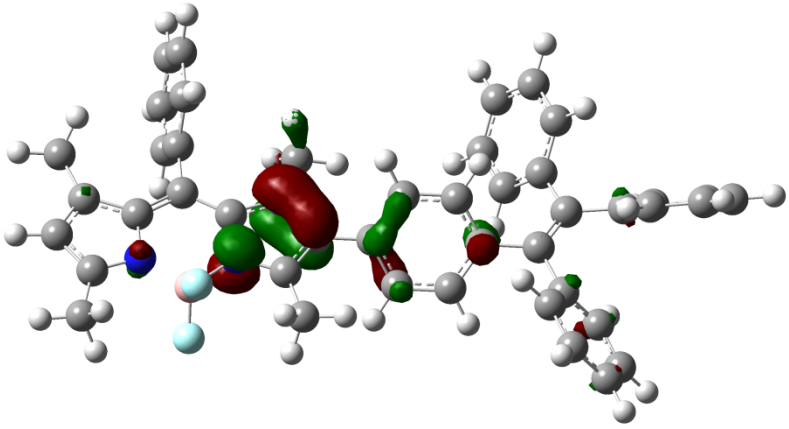


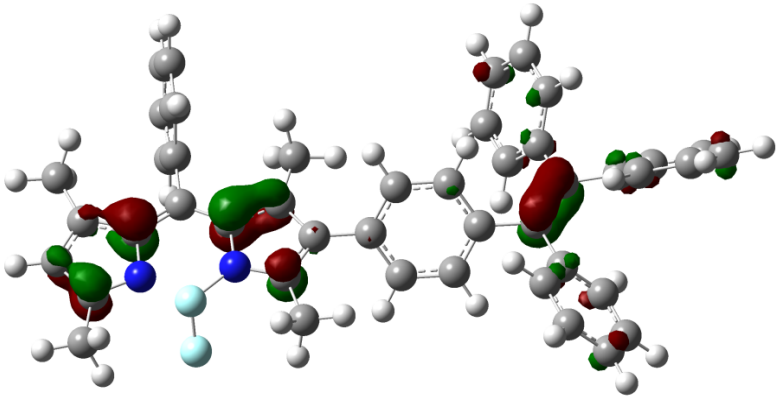
Figure S10. Cyclic voltammograms of **1**–**4** (1.0 mM) in CH_2Cl_2. Scan rate = 0.1 V/s.

Table S1. Calculated electronic excitation energies, oscillator strengths and the related wave function

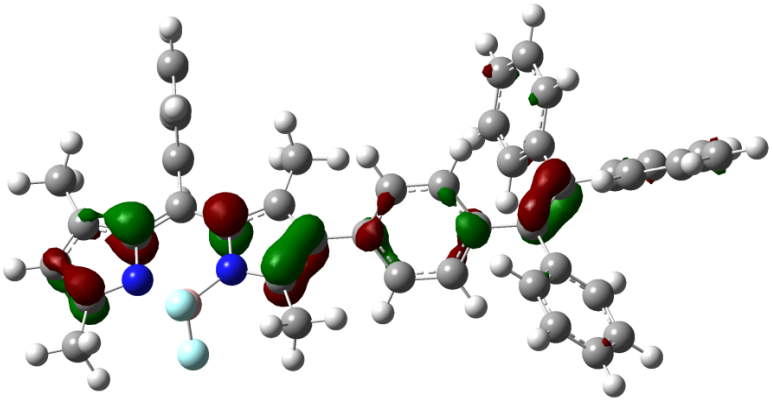
Dyes	State	Energy[eV]	λ[nm]	*f*	Orbitals(Coefficient)
1	S_1	2.5521	485.82	0.1914	H–L(0.63960) H-1–L(0.28229)
	S_2	2.9645	418.23	0.5885	H–L(-0.25106) H-1–L(0.63210)
	S_3	3.3307	372.24	0.2238	H–L(0.15725) H-2–L(0.64684)
	S_4	3.5235	351.88	0.1709	H–L+1(0.64904) H-4–L(0.14694)
2	S_1	2.4673	502.51	0.4928	H–L(0.66693) H-2–L(0.20111)
	S_2	2.5956	477.67	0.0115	H-1–L(0.70379)
	S_3	2.9162	425.16	0.7040	H-2–L(0.66199) H–L(-0.17005)
	S_4	3.2871	377.19	0.3659	H-3–L(0.65740) H–L(0.13488)
3	S_1	2.4356	509.06	0.5573	H–L(0.68030) H-2–L+1(-0.16376)
	S_2	2.4788	500.17	0.0015	H-1–L(0.57846) H–L+1(-0.31355)
	S_3	2.5351	489.07	0.2904	H-1–L+1(0.63763) H-2–L(0.28297)
	S_4	2.5450	487.17	0.0123	H–L+1(0.52690) H-1–L(0.31411)



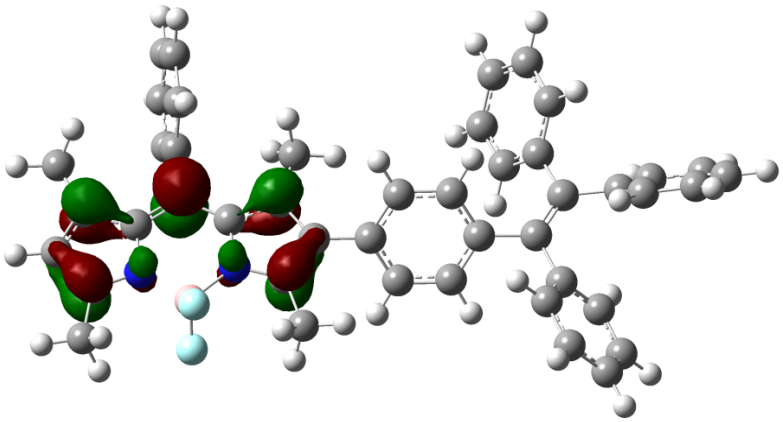
HOMO-2 (-6.20 eV)



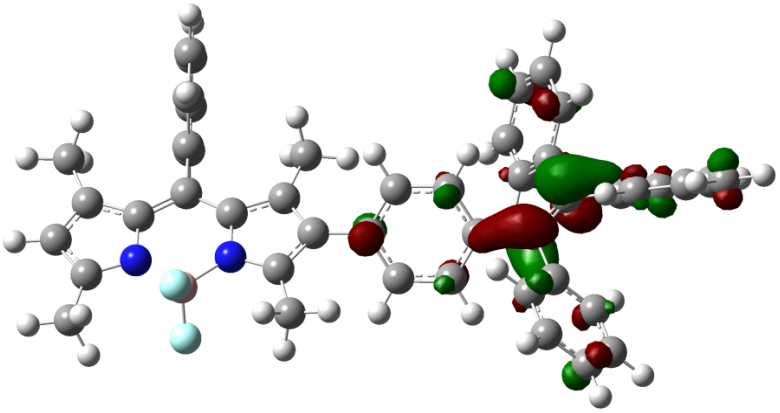
HOMO-1 (-5.43 eV)



HOMO (-5.19 eV)

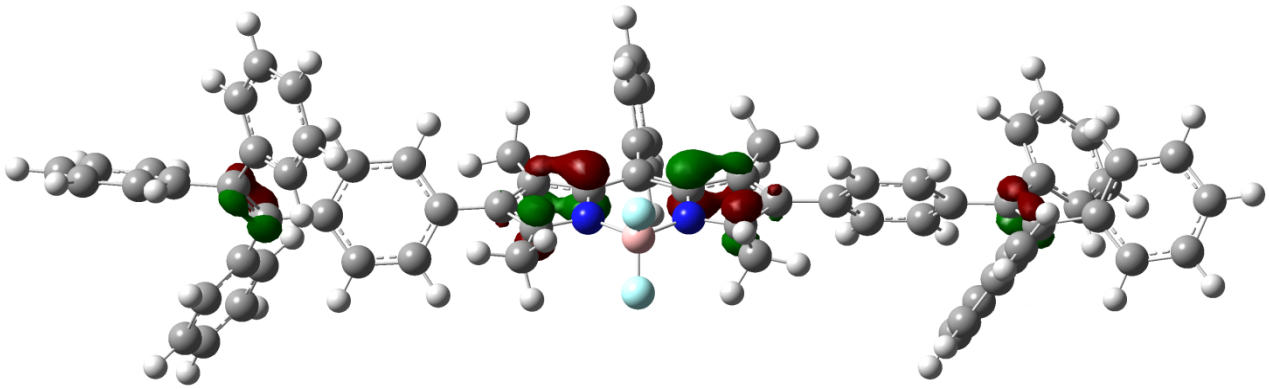


LUMO (-2.36 eV)

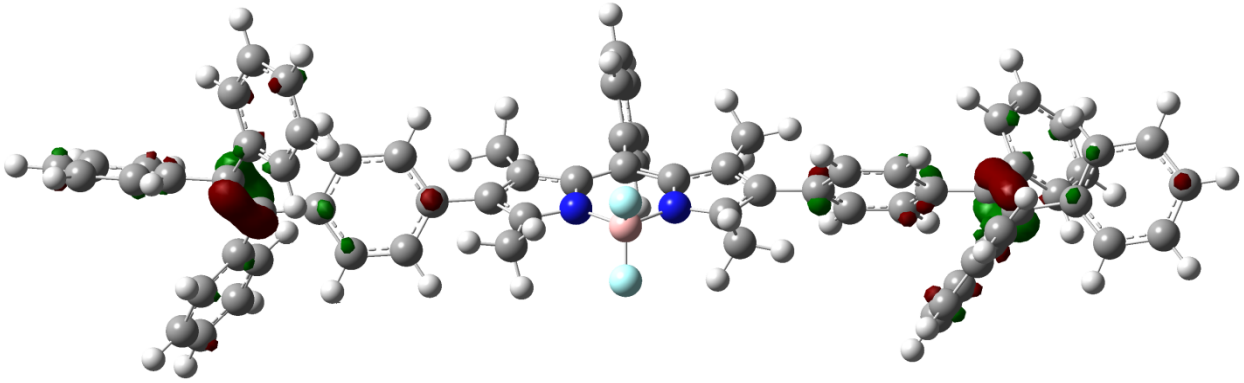


LUMO+1 (-1.26 eV)

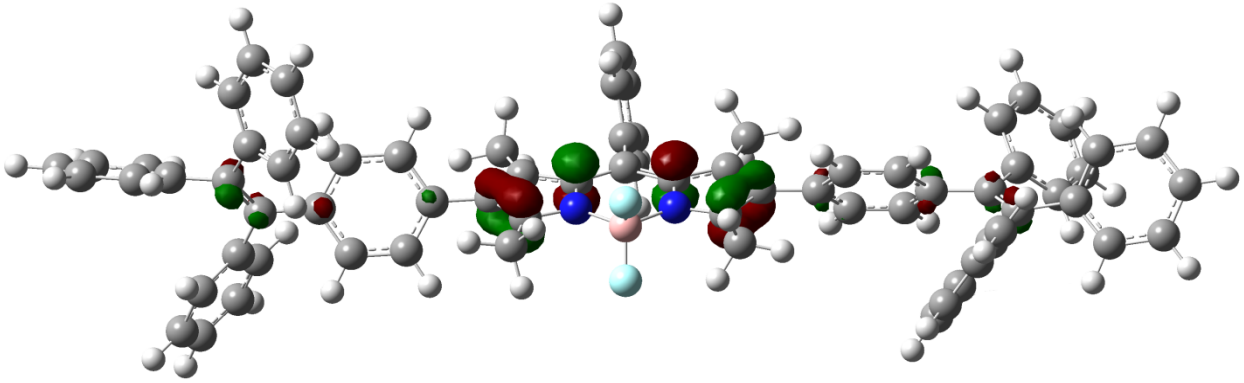
Figure S11. Some frontier π MOs energy levels of compound **1**.



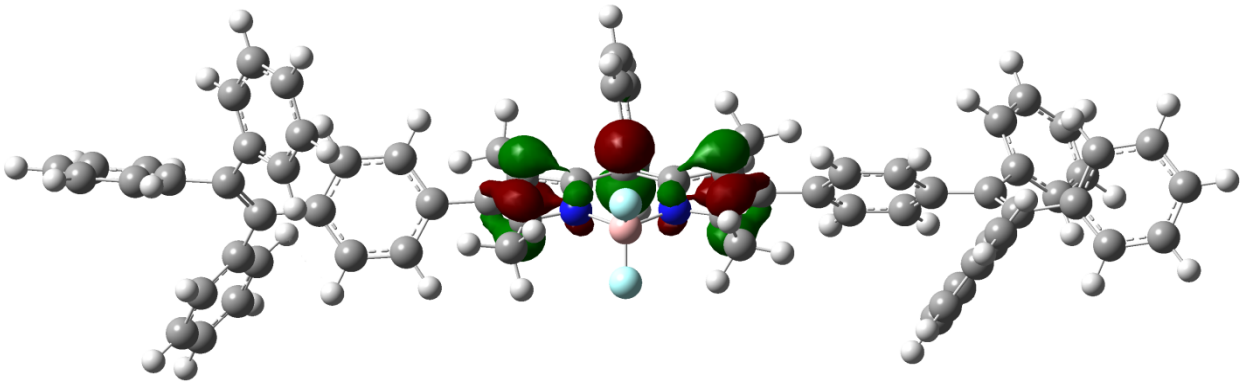
HOMO-2 (-5.46 eV)



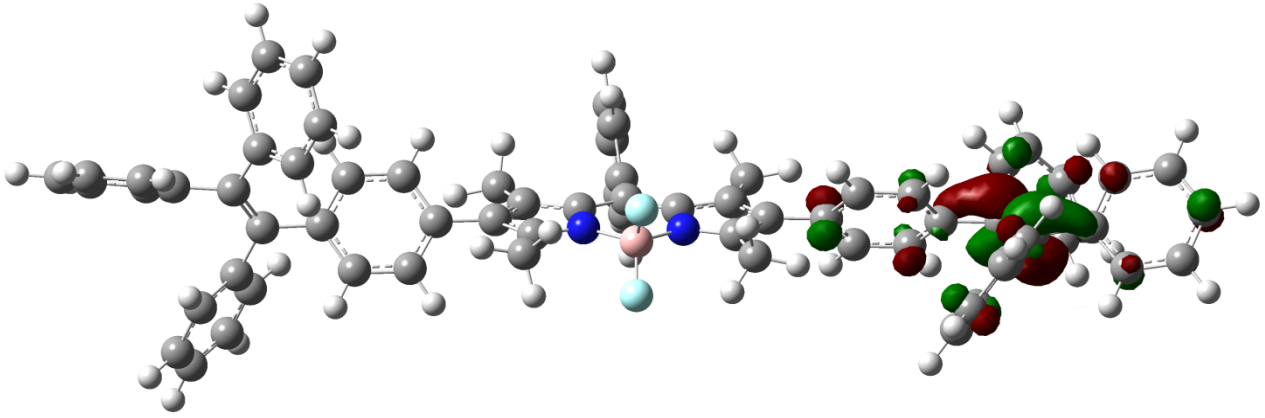
HOMO-1 (-5.31 eV)



HOMO (-5.12 eV)

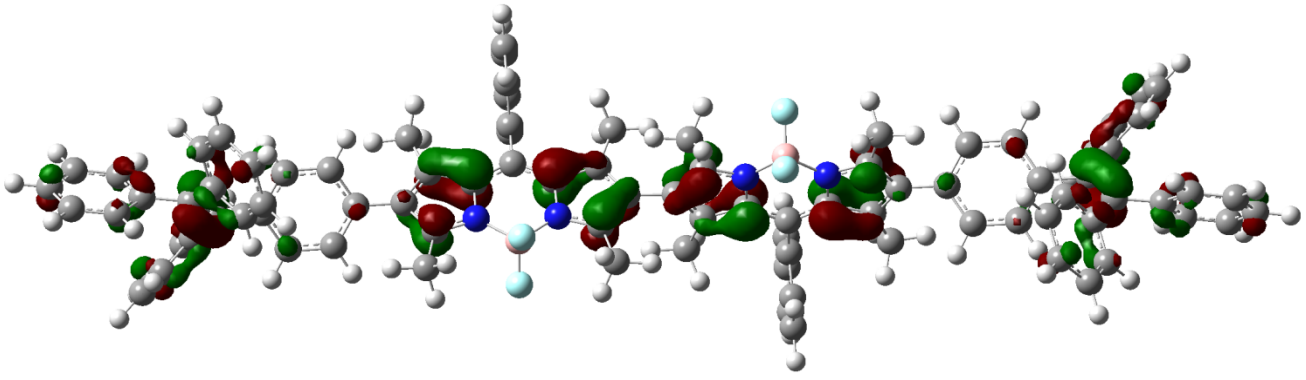


LUMO (-2.37 eV)

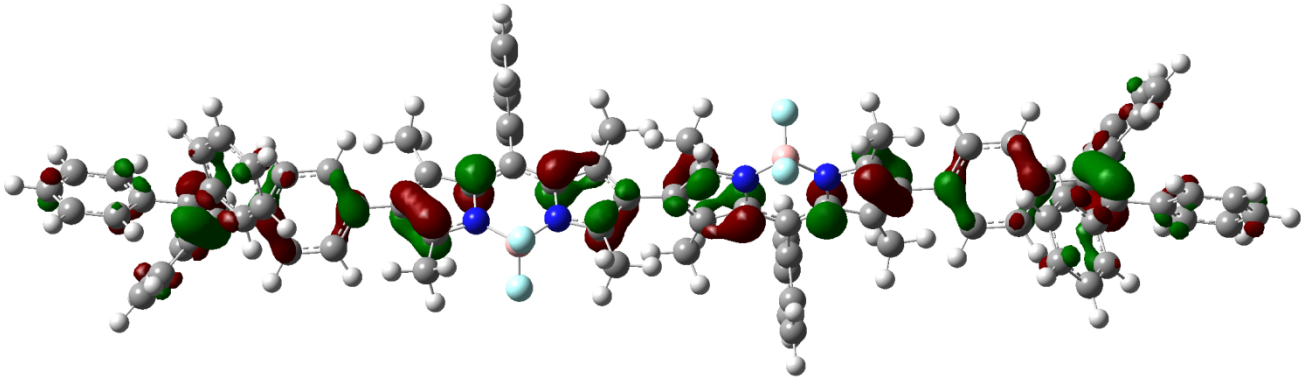


LUMO+1 (-1.26 eV)

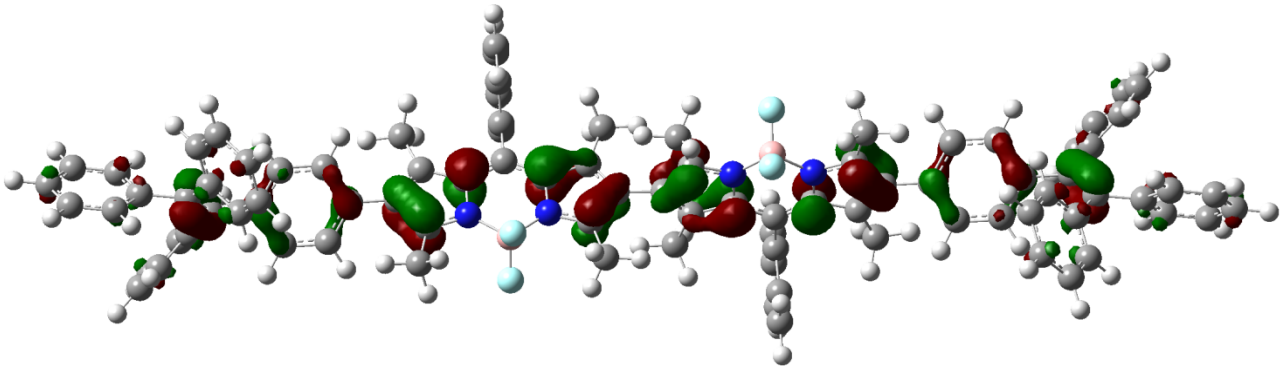
Figure S12. Some frontier π MOs energy levels of compound **2**.



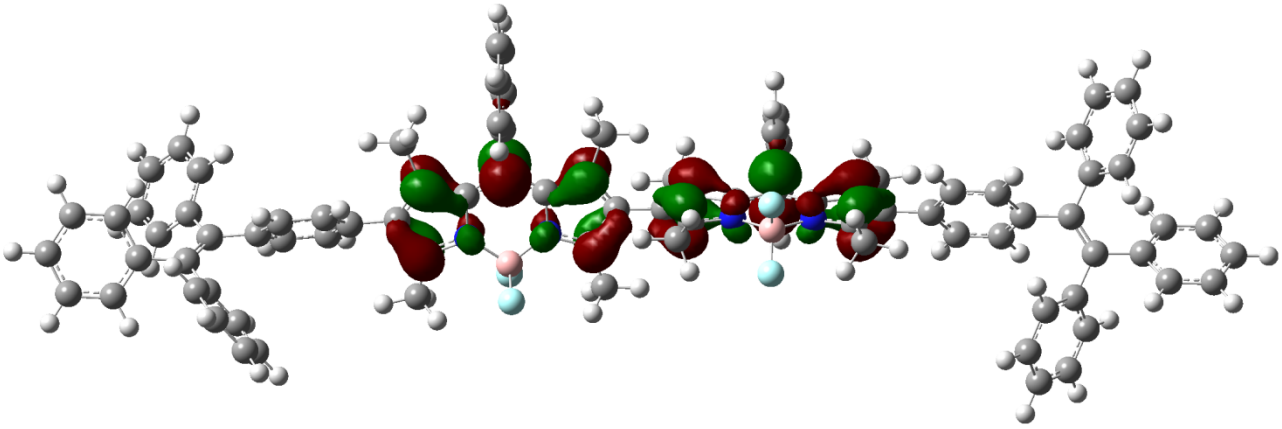
HOMO-2 (-5.43 eV)



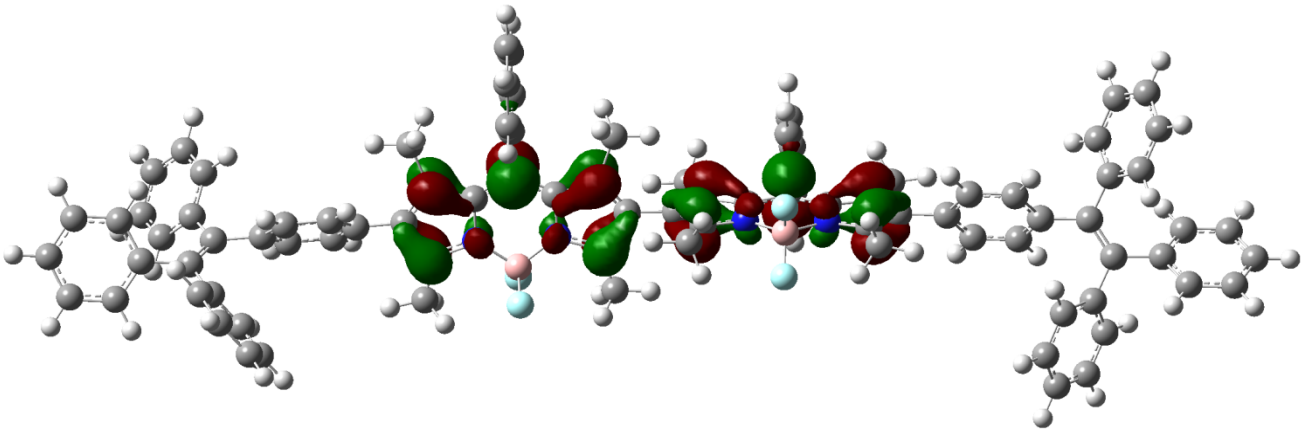
HOMO-1 (-5.21 eV)



HOMO (-5.18 eV)



LUMO (-2.43 eV)



LUMO+1 (-2.34 eV)

Figure S13. Some frontier π MOs energy levels of compound **3**.