

ESI for

Synthesis, characterization and properties of furan-containing difluoroboron complexes

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Content

X-ray Structural Analysis and Summary of crystal data. *Page S3- S4*

NMR and MS Spectra for Ligands and BF₂ Complexes *Page S5- S21*

References *Page S21*

X-ray Structural Analysis

Crystals suitable were grown by slow diffusion of n-hexane into the respective solutions of **F2** or **F3** in chloroform at room temperature. Reflection data were collected at 296 (2) K using a graphite monochromator with Mo-K α radiation ($\lambda = 0.71073$ Å) on a Bruker SMART APEX(II) CCD diffractometer. The collected frames were processed with the software SAINT and an absorption correction (SADABS) was used to the collected reflections. The resulting structure was solved by the Direct or Patterson methods (SHELXTL 97) in conjunction with standard difference Fourier techniques and then refined by full-matrix least-square technique on F^2 . All hydrogen atoms were positioned geometrically and non-hydrogen atoms were refined anisotropically. Relevant crystal data for the structures are collected in Table S1.

CCDC-1486089 (for **F2**), 1482992 (for **F3**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Summary of crystal data.

Complexes	F2	F3
CCDC number	1486089	1482992
Moiety formula	C ₂₃ H ₁₅ BF ₂ O ₃	C ₂₀ H ₁₅ BF ₂ O ₄
formula weight	388.16	368.13
temperature, K	296(2)	296(2)
wavelength (Å)	0.71073	0.71073
crystal system	Monoclinic	Triclinic
space group	P2(1)/c	P-1
unit cell dimensions		
a (Å)	16.880	8.808
b (Å)	9.056	13.609
c (Å)	11.782	14.247
α (deg)	90	76.62
β (deg)	97.50	87.56
γ (deg)	90	88.26
volume (Å ³)	1785.6	1659.6
Z	4	4
density, calcd (g/cm ³)	1.444	1.473
Absorption coefficient(mm ⁻¹)	0.108	0.115
F(000)	800	760
θ range for data collection(deg)	2.43-25.00	2.36-27.52
reflections collected	8561 / 3136 [R(int) = 0.0436]	12058 / 7508 [R(int) = 0.1034]
refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
data/restraints/parameters	3136 / 0 / 262	7508 / 0 / 487
goodness-of-fit on F^2 [a]	1.017	1.042
final R indices [$I > 2\sigma(I)$] [b]	0.0517	0.0535
R indices (all data)	0.0879	0.0638

$$[\text{a}] \text{ goodness - of - fit} = \left\{ \left(\frac{\sum [w(F_0^2 - F_C^2)^2]}{N_{\text{obs}} - N_{\text{param}}} \right) \right\}^{1/2}$$

$$[\text{b}] R_1 = \frac{\sum |F_0| - |F_C|}{\sum |F_0|}. \quad \text{wR2} = \left\{ \frac{\sum [w(F_0^2 - F_C^2)^2]}{\sum [w(F_0^2)^2]} \right\}^{1/2}$$

NMR and MS Spectra for Ligands and BF₂ Complexes

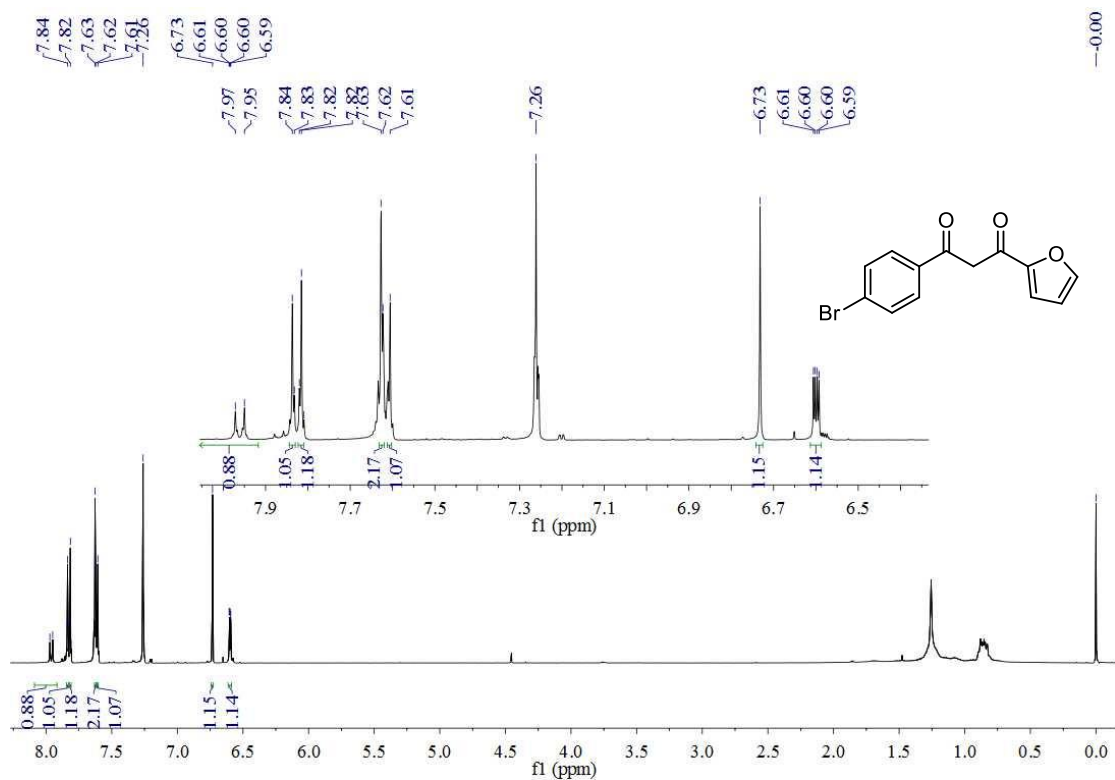


Figure S1. The ¹H NMR spectrum of Compound 3 in CDCl₃.

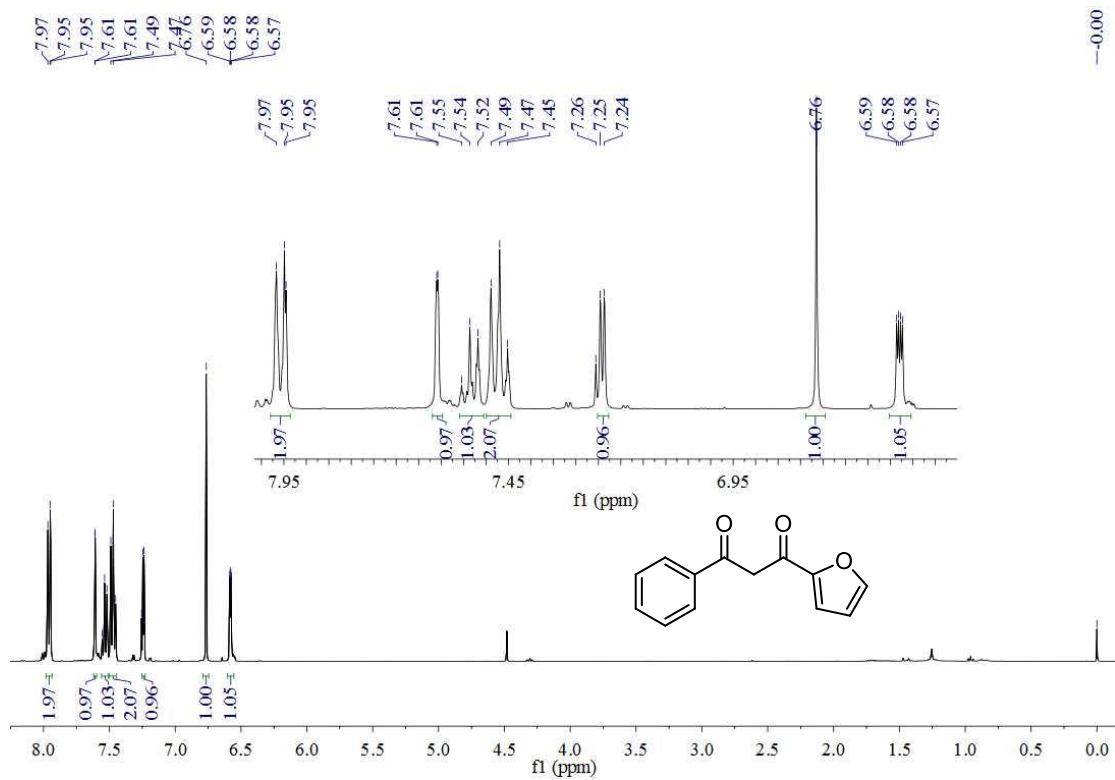


Figure S2. The ¹H NMR spectrum of Ligand LF0 in CDCl₃.

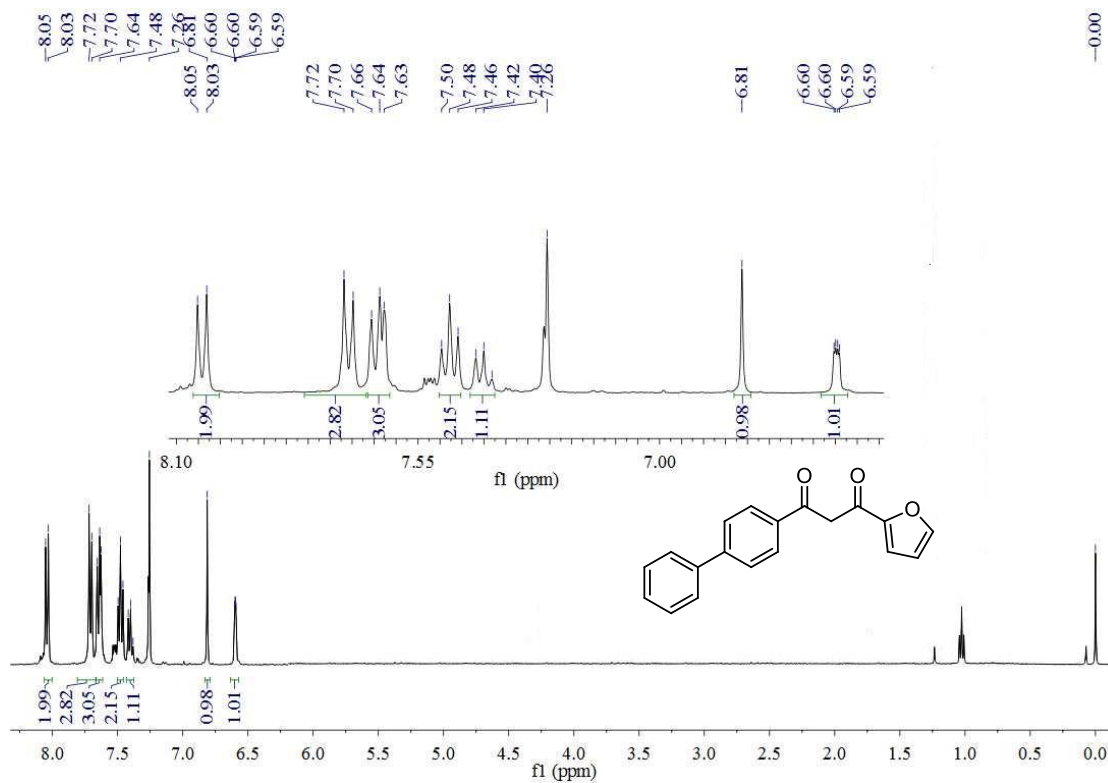


Figure S3. The ^1H NMR spectrum of Ligand LF1 in CDCl_3 .

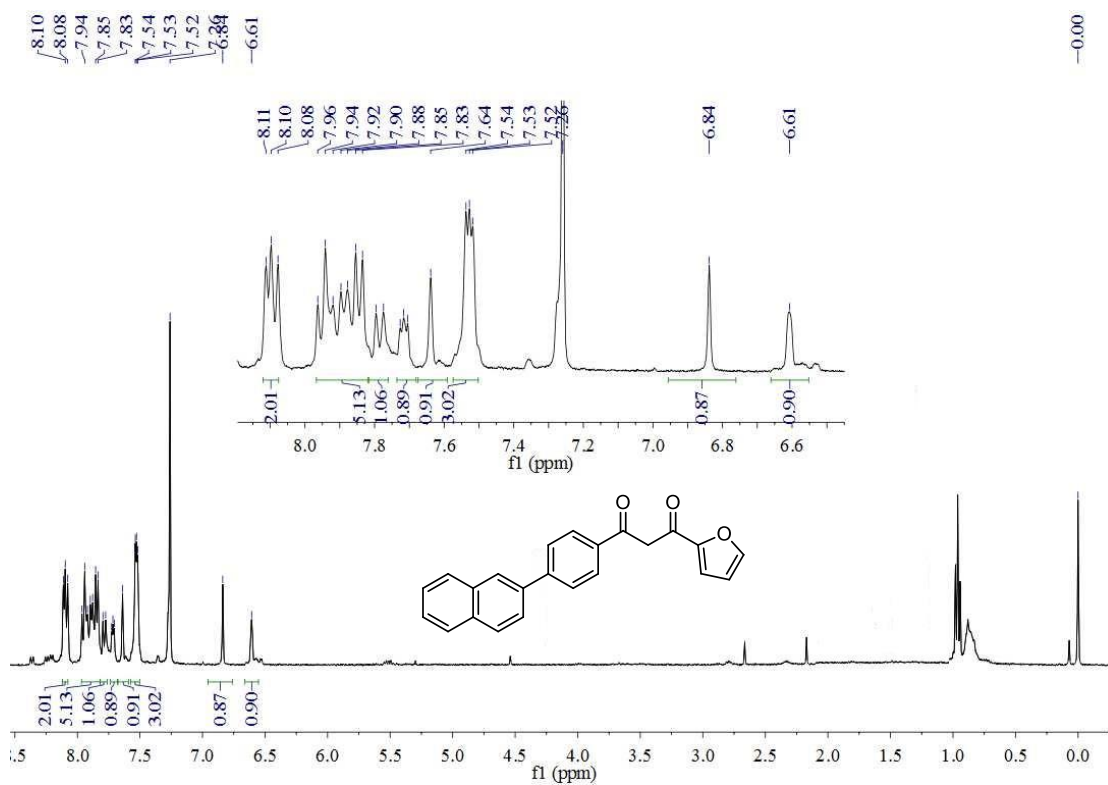


Figure S4. The ^1H NMR spectrum of Ligand LF2 in CDCl_3 .

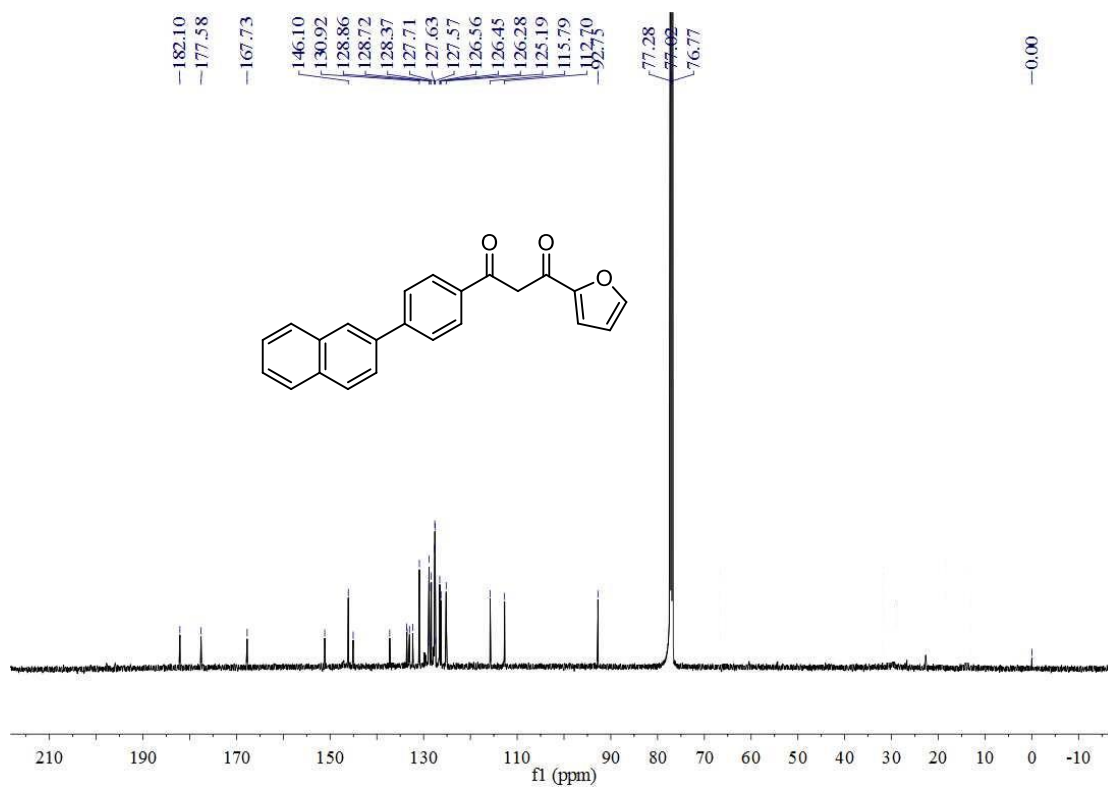


Figure S5. The ^{13}C NMR spectrum of Ligand LF2 in CDCl_3 .

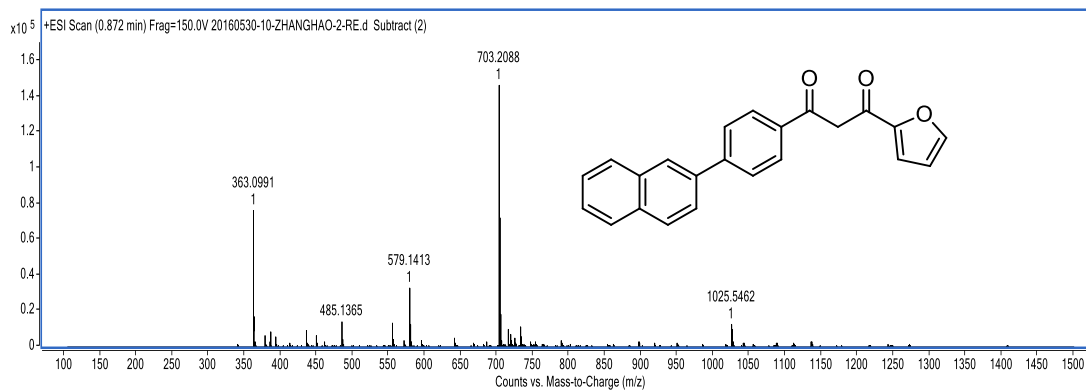


Figure S6. The HRMS spectrum of Ligand LF2.

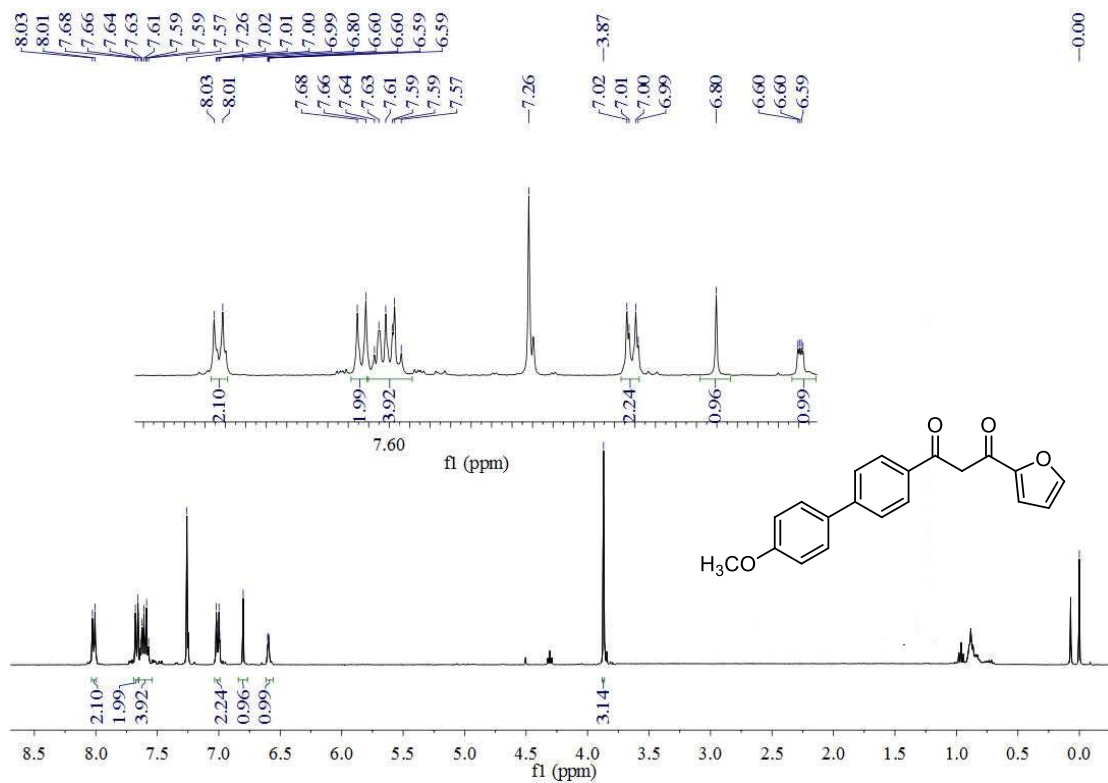


Figure S7. The ¹H NMR spectrum of Ligand LF3 in CDCl₃.

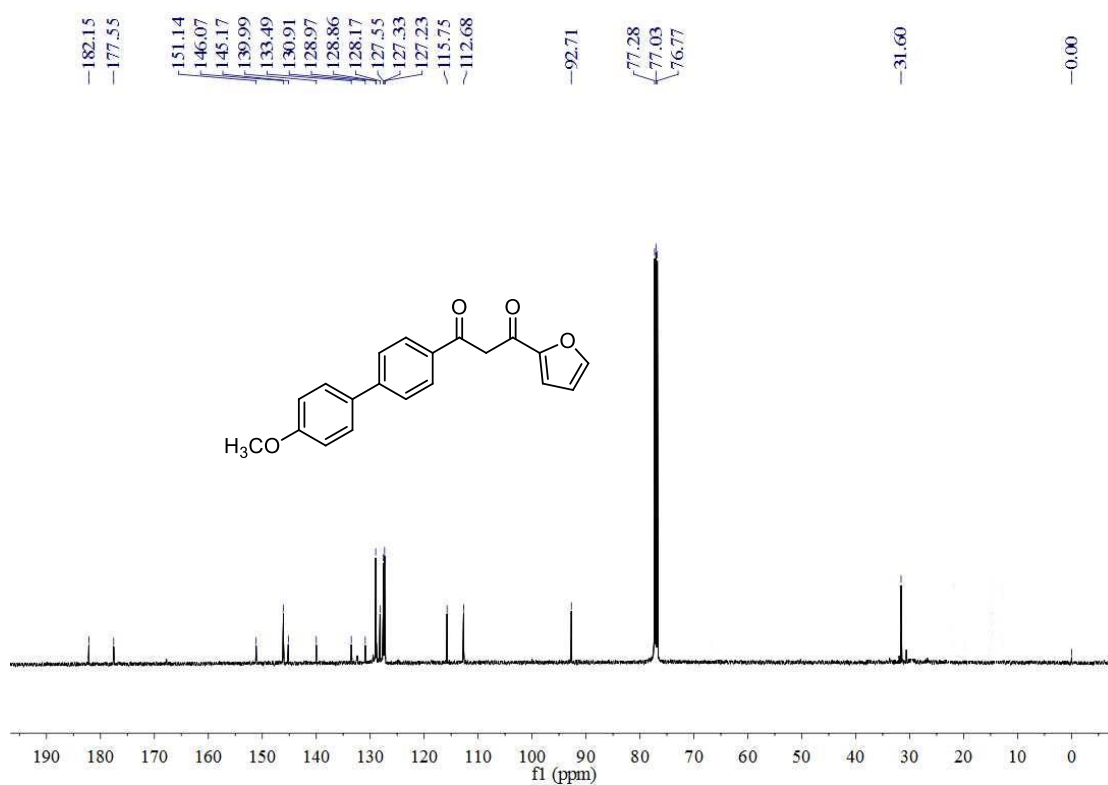


Figure S8. The ¹³C NMR spectrum of Ligand LF3 in CDCl₃.

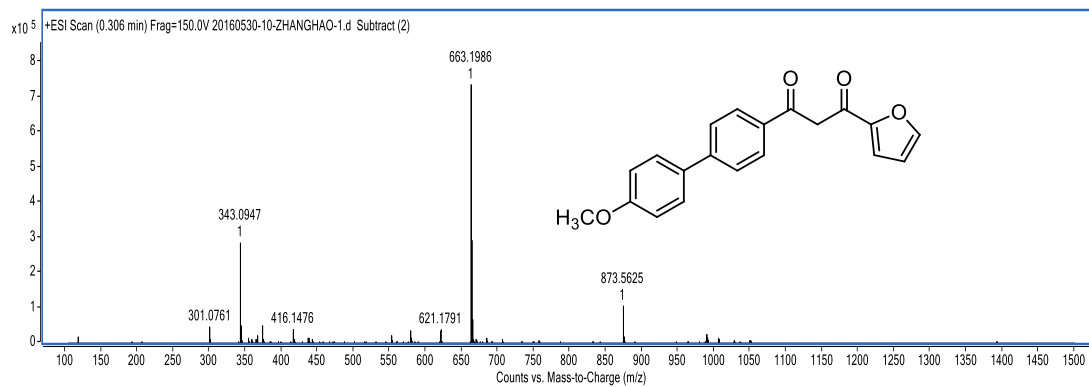


Figure S9. The HRMS spectrum of Ligand LF3.

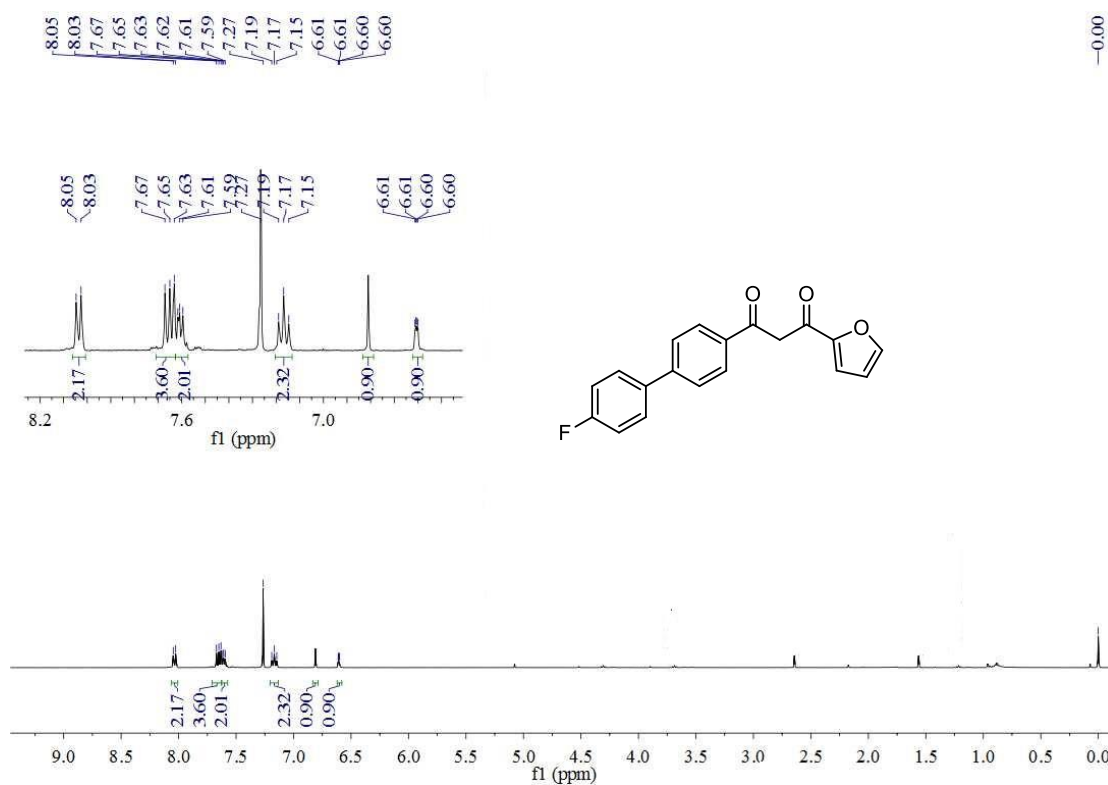


Figure S10. The ^1H NMR spectrum of Ligand LF4 in CDCl_3 .

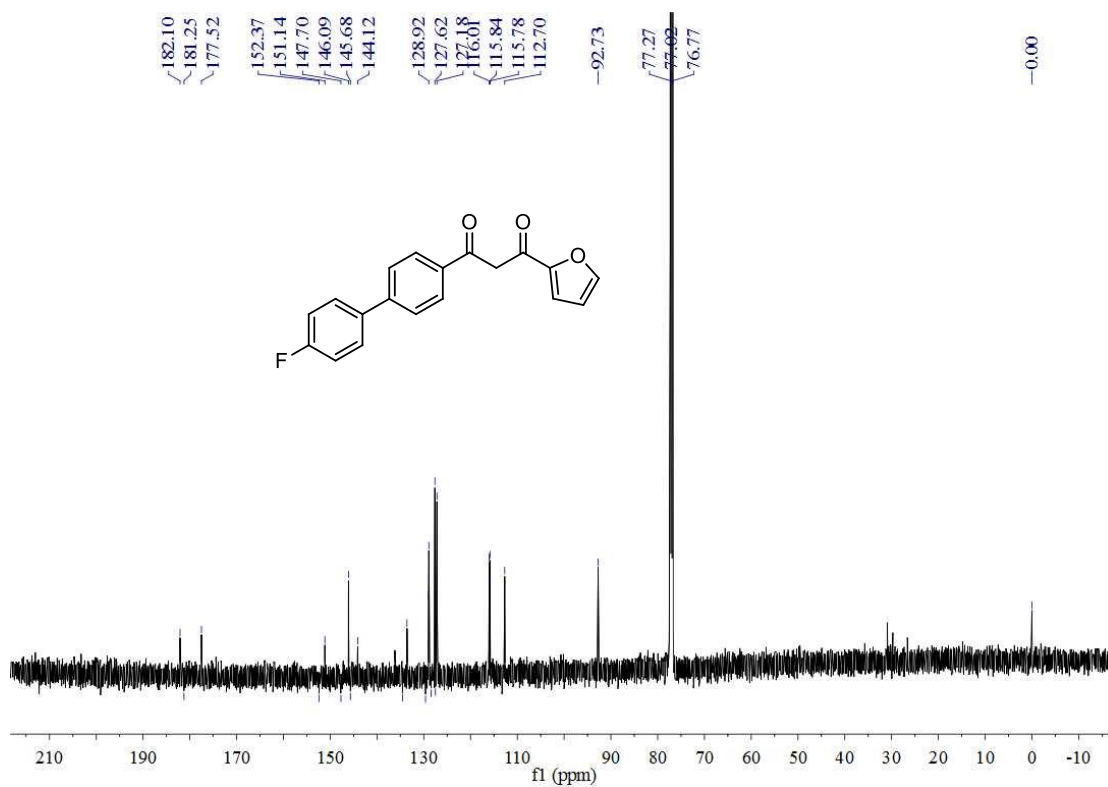


Figure S11. The ^{13}C NMR spectrum of Ligand LF4 in CDCl_3 .

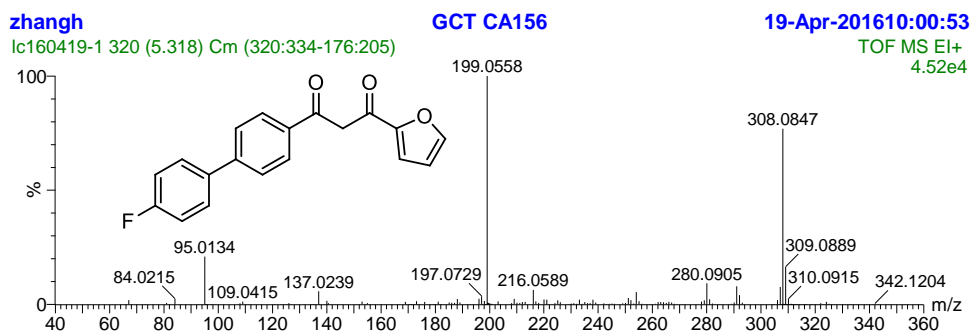


Figure S12. The HRMS spectrum of Ligand LF4.

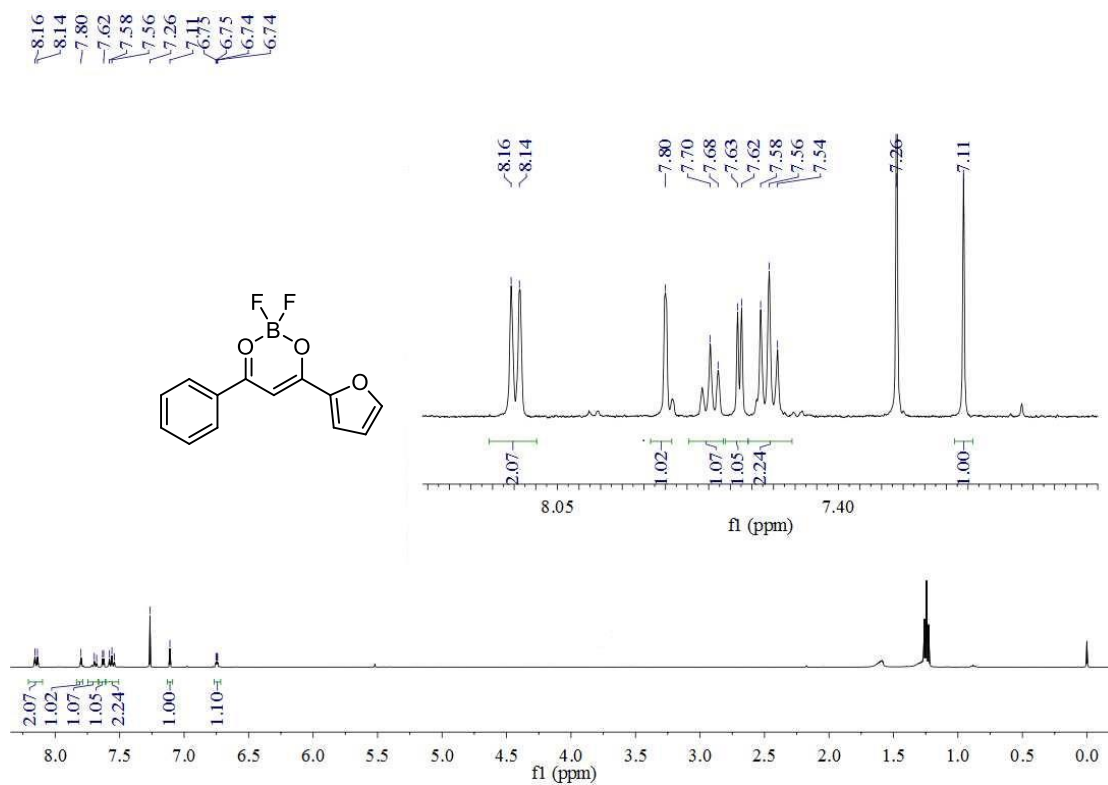


Figure S13. The ¹H NMR spectrum of complex **F0** in CDCl₃.

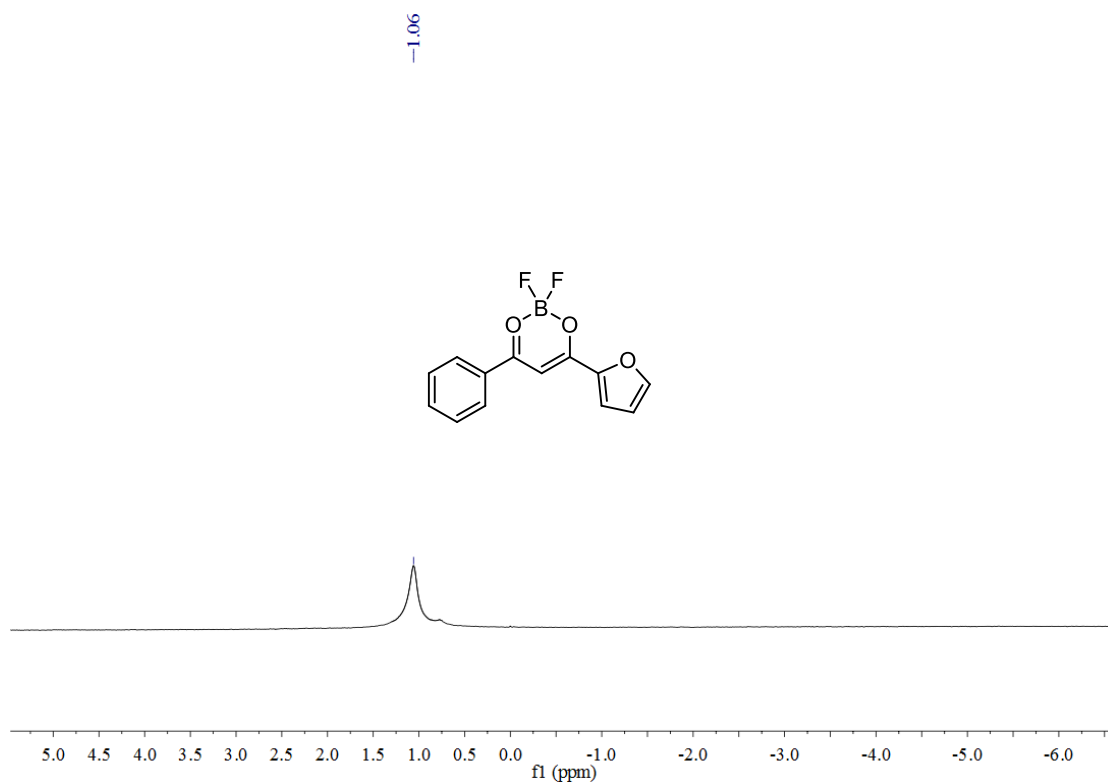


Figure S14. The ¹¹B NMR spectrum of complex **F0** in CDCl₃.

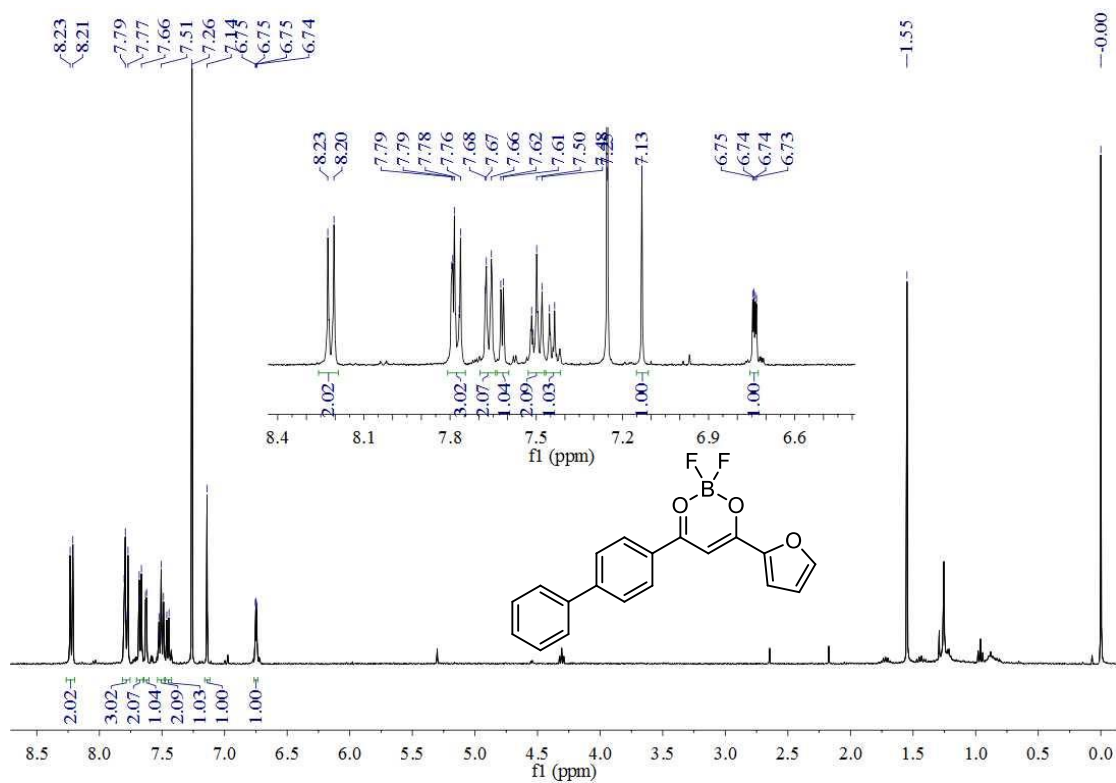


Figure S15. The ¹H NMR spectrum of complex F1 in CDCl₃.

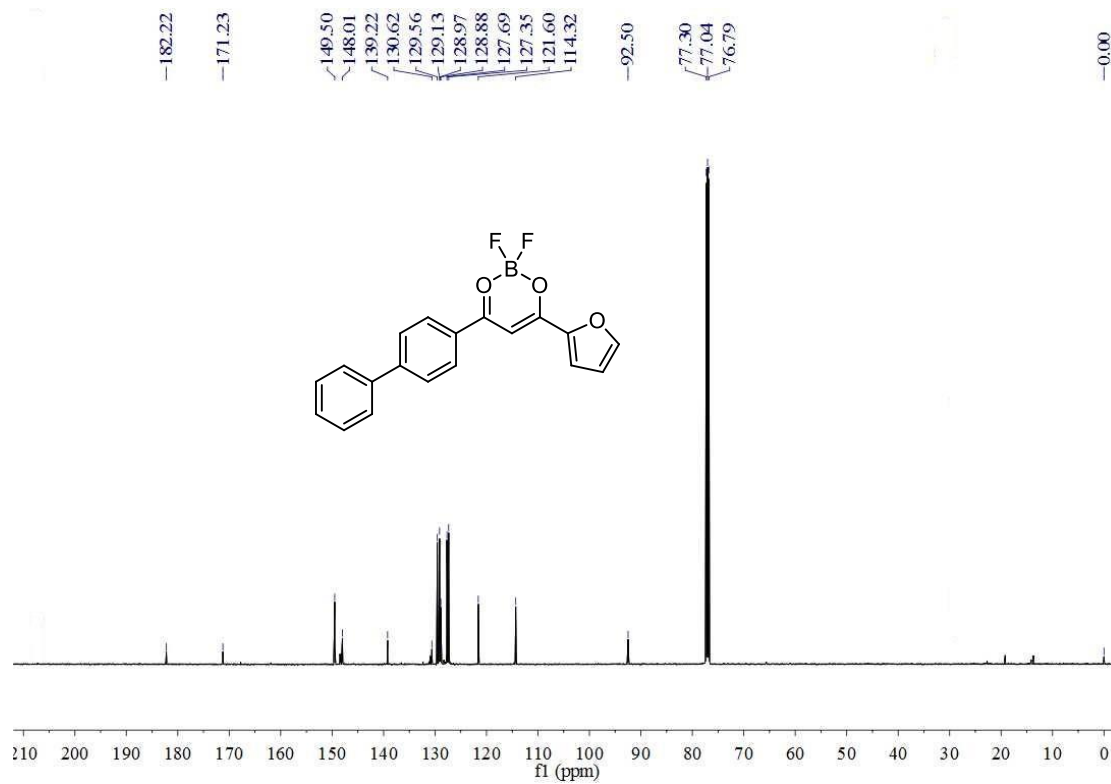


Figure S16. The ¹³C NMR spectrum of complex F1 in CDCl₃.

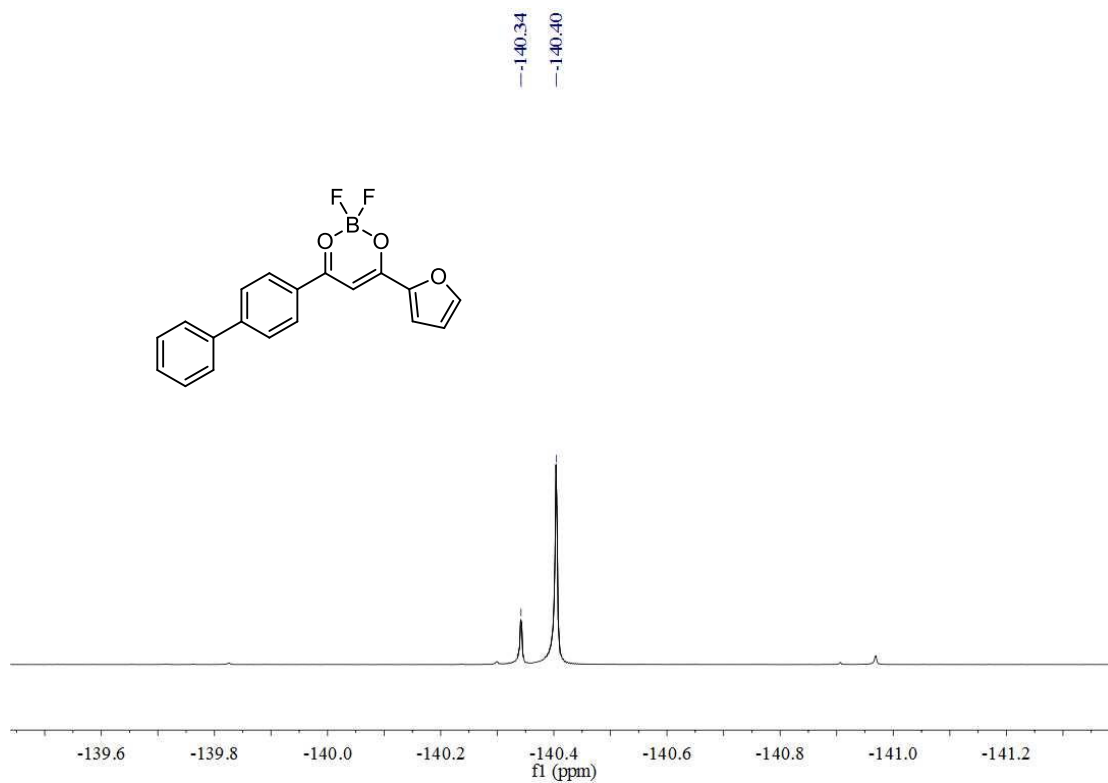


Figure S17. The ^{19}F NMR spectrum of complex F1 in CDCl_3 .

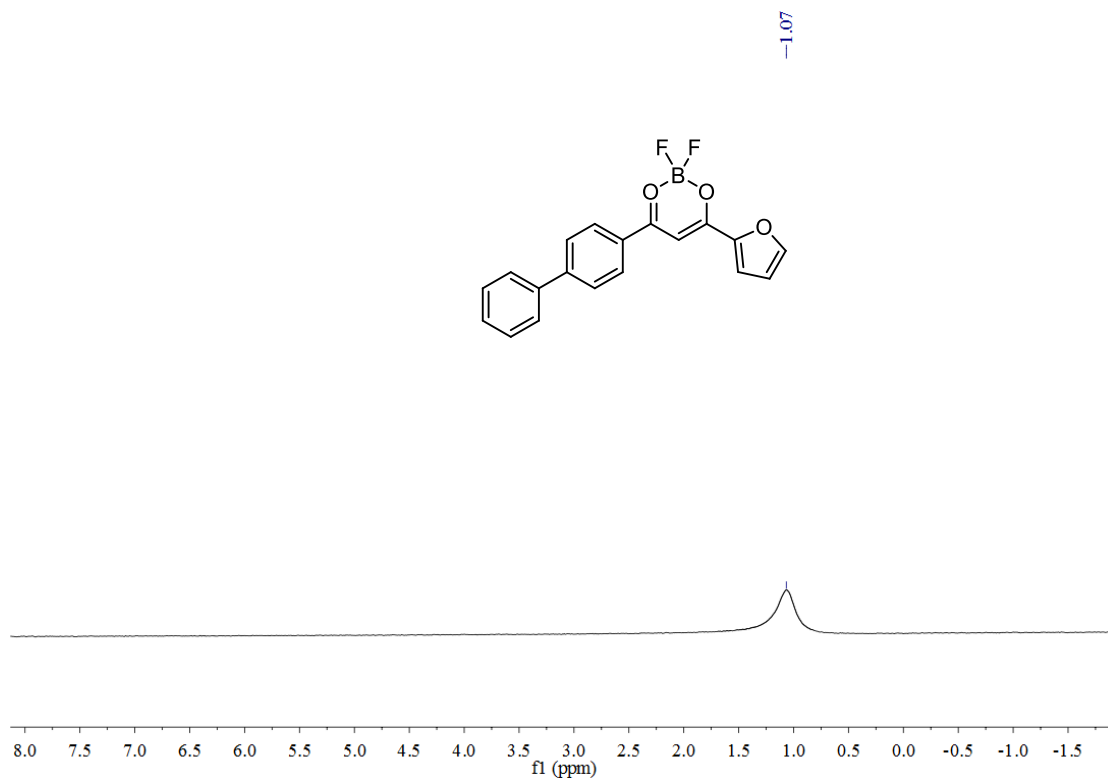


Figure S18. The ^{11}B NMR spectrum of complex F1 in CDCl_3 .

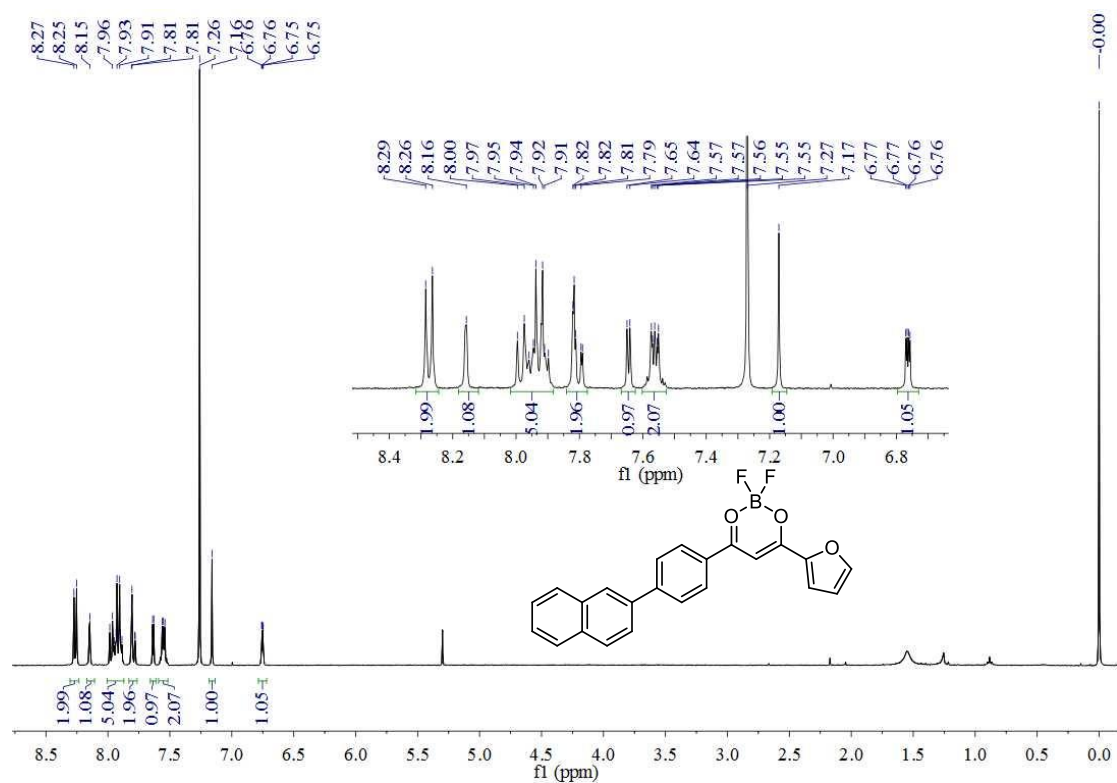
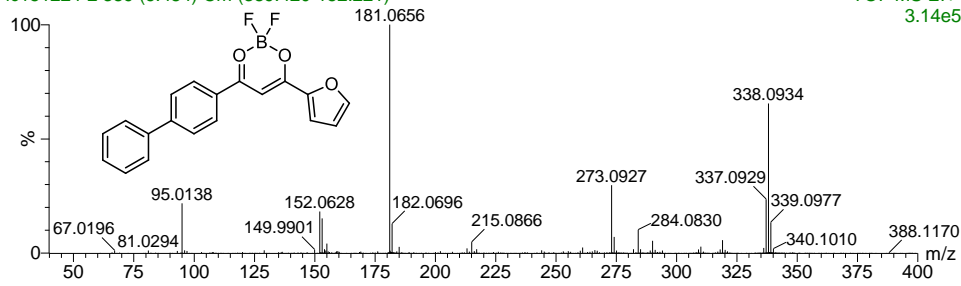
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3.14e5



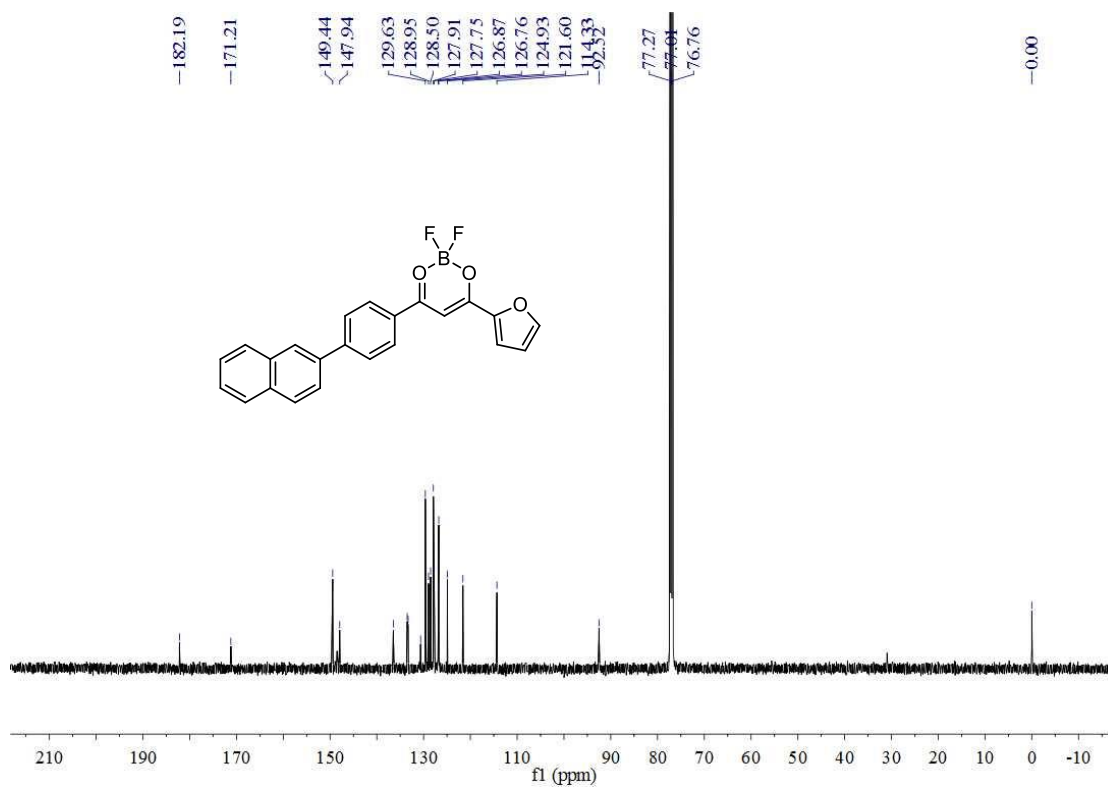


Figure S21. The ¹³C NMR spectrum of complex F2 in CDCl₃.

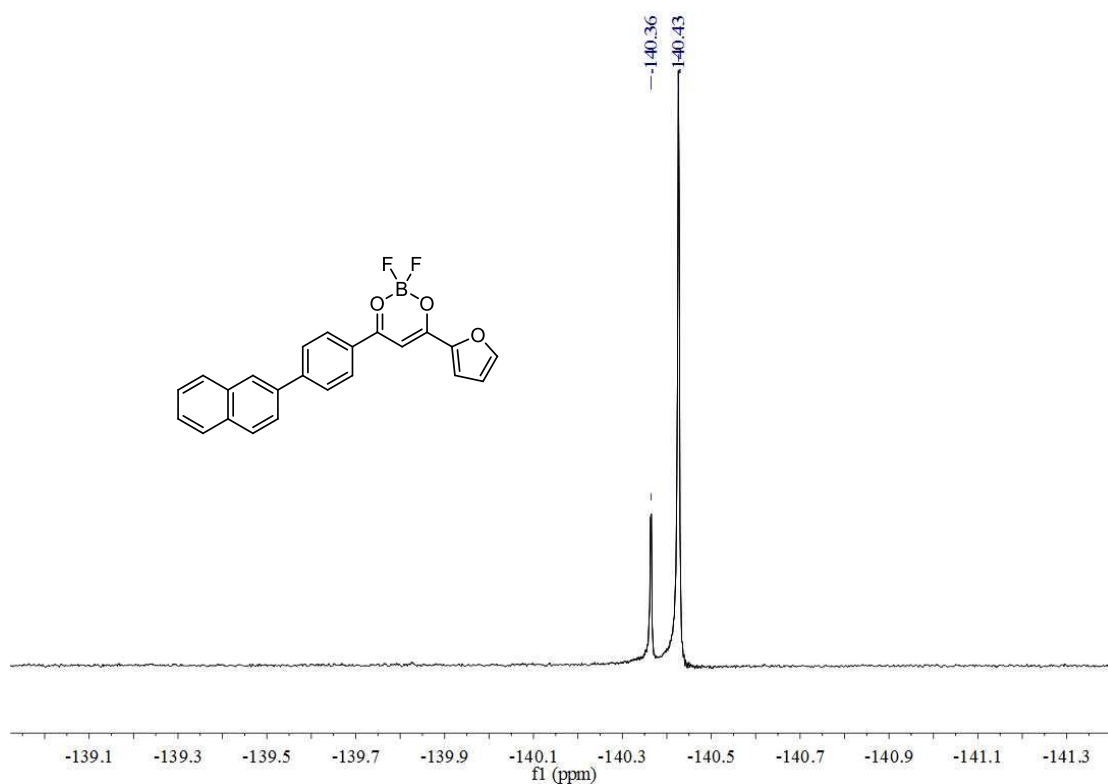


Figure S22. The ¹⁹F NMR spectrum of complex F2 in CDCl₃.

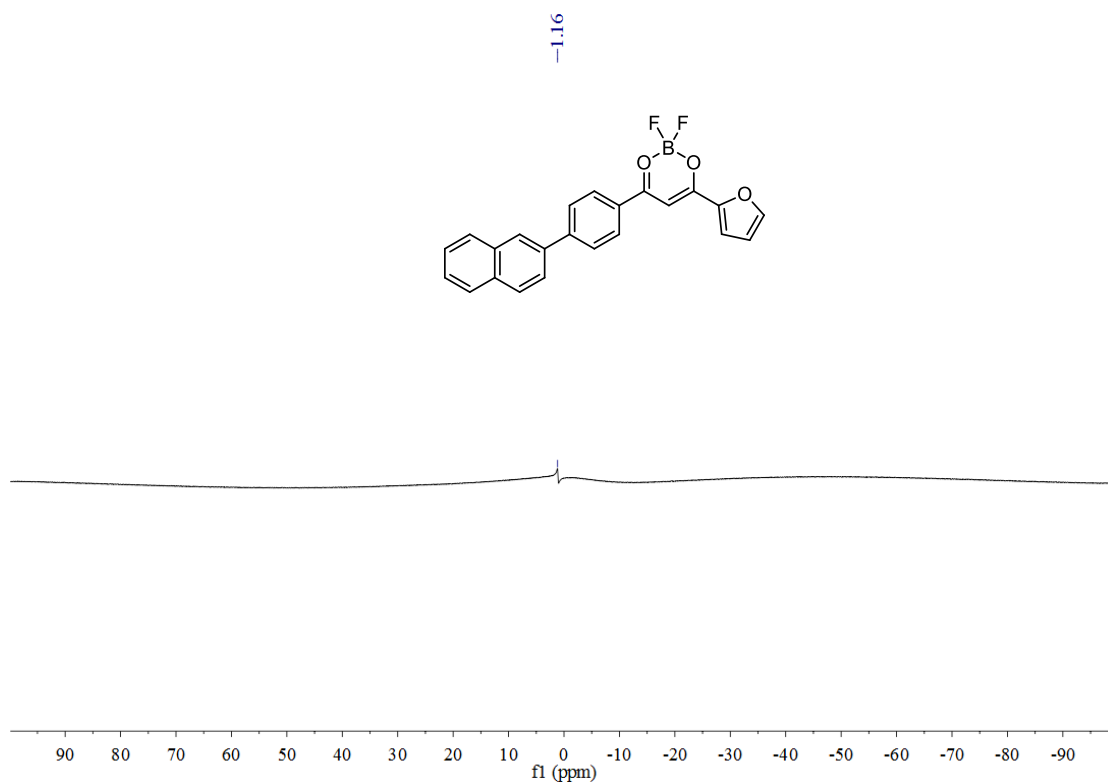


Figure S23. The ^{11}B NMR spectrum of complex **F2** in CDCl_3 .

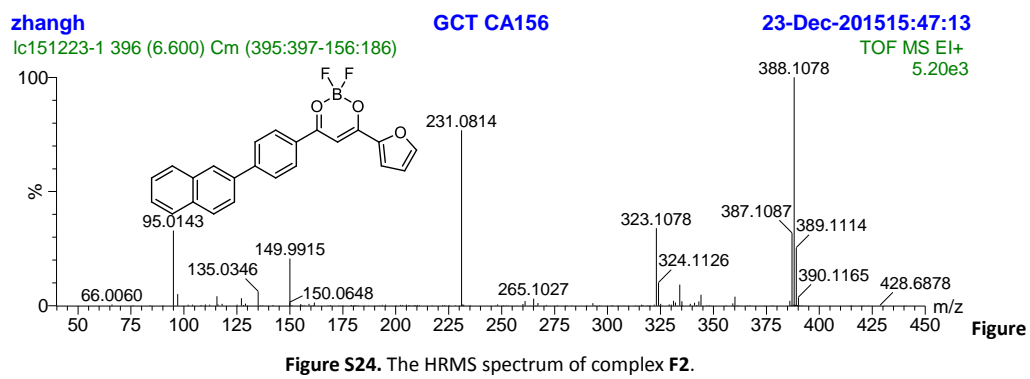


Figure S24. The HRMS spectrum of complex **F2**.

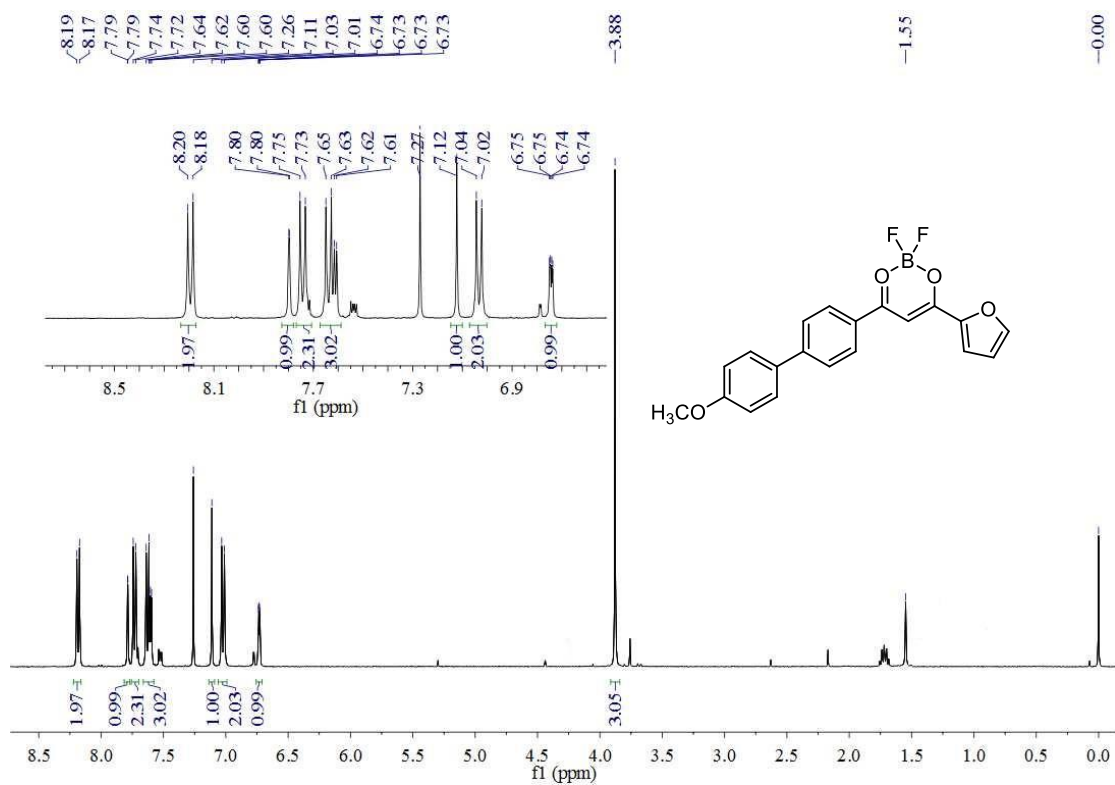


Figure S25. The ¹H NMR spectrum of complex F3 in CDCl₃.

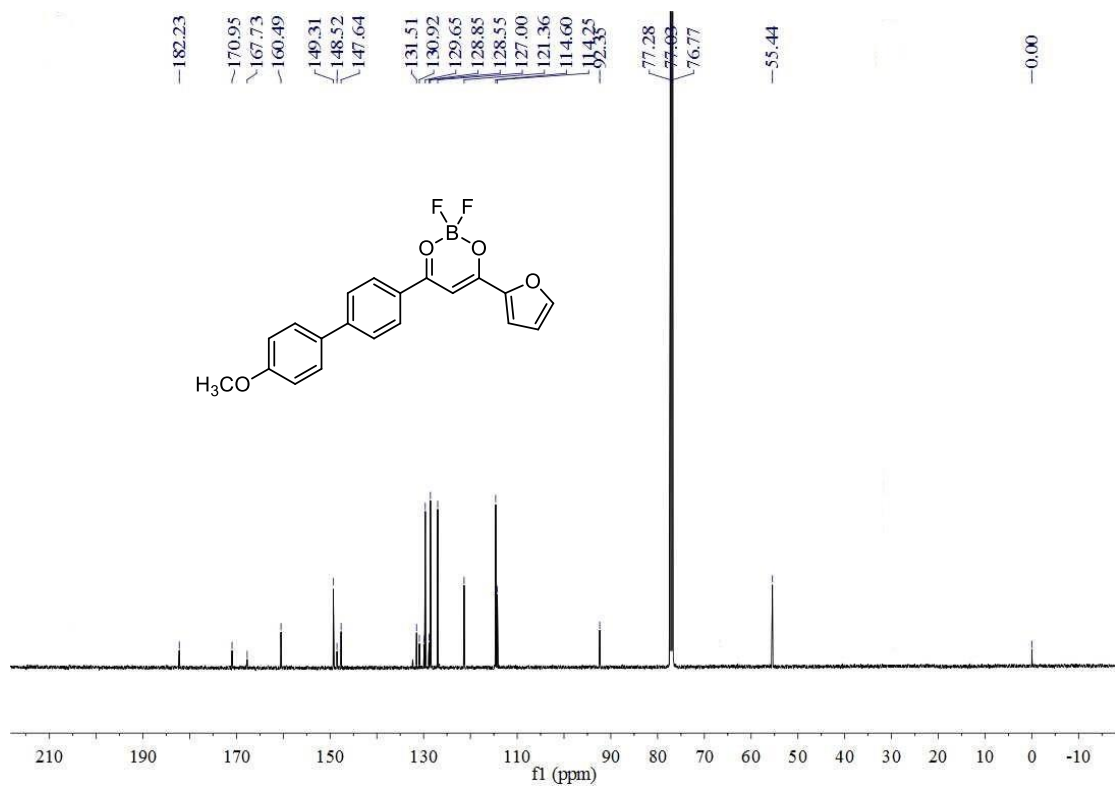


Figure S26. The ¹³C NMR spectrum of complex F3 in CDCl₃.

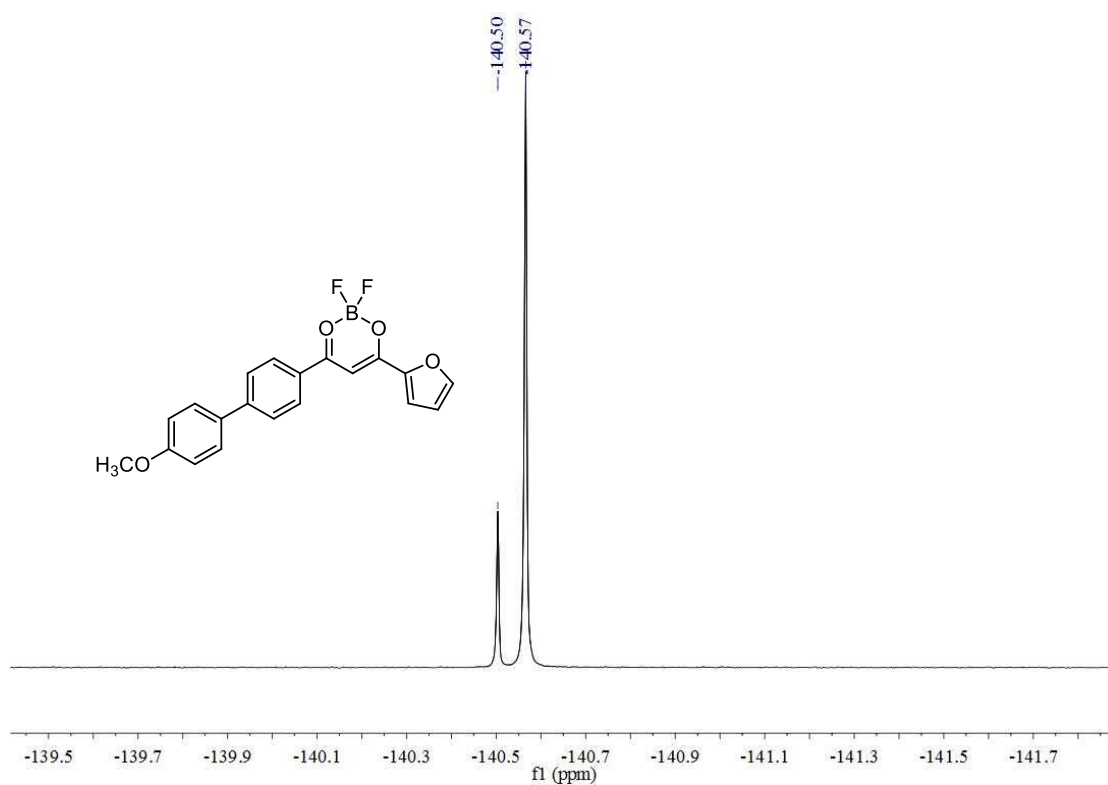


Figure S27. The ^{19}F NMR spectrum of complex **F3** in CDCl_3 .

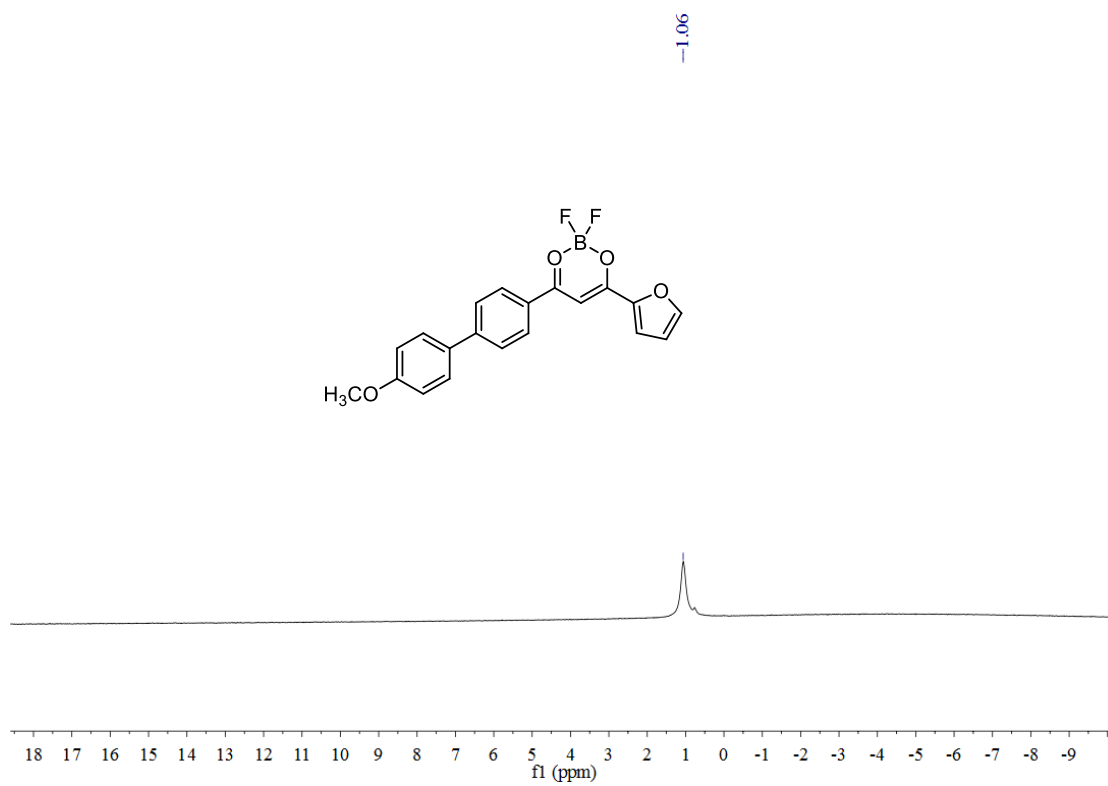


Figure S28. The ^{11}B NMR spectrum of complex **F3** in CDCl_3 .

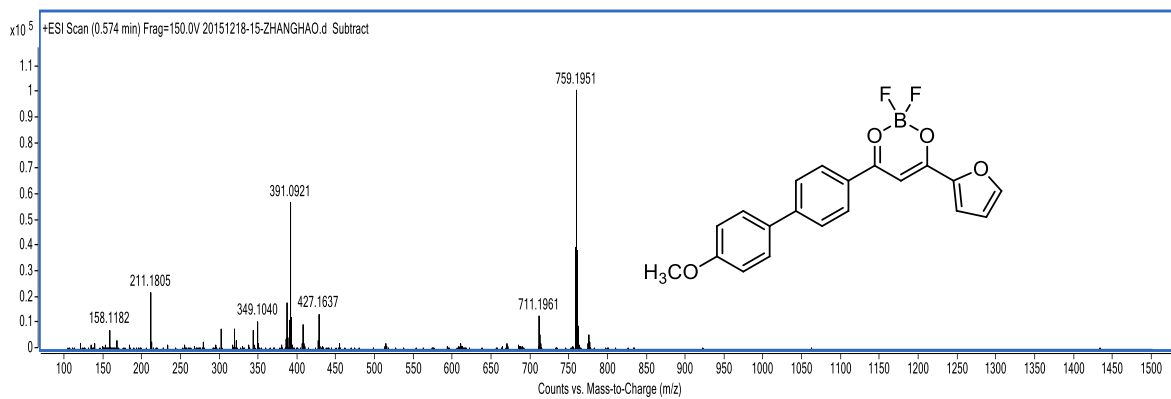


Figure S29. The HRMS spectrum of complex F3.

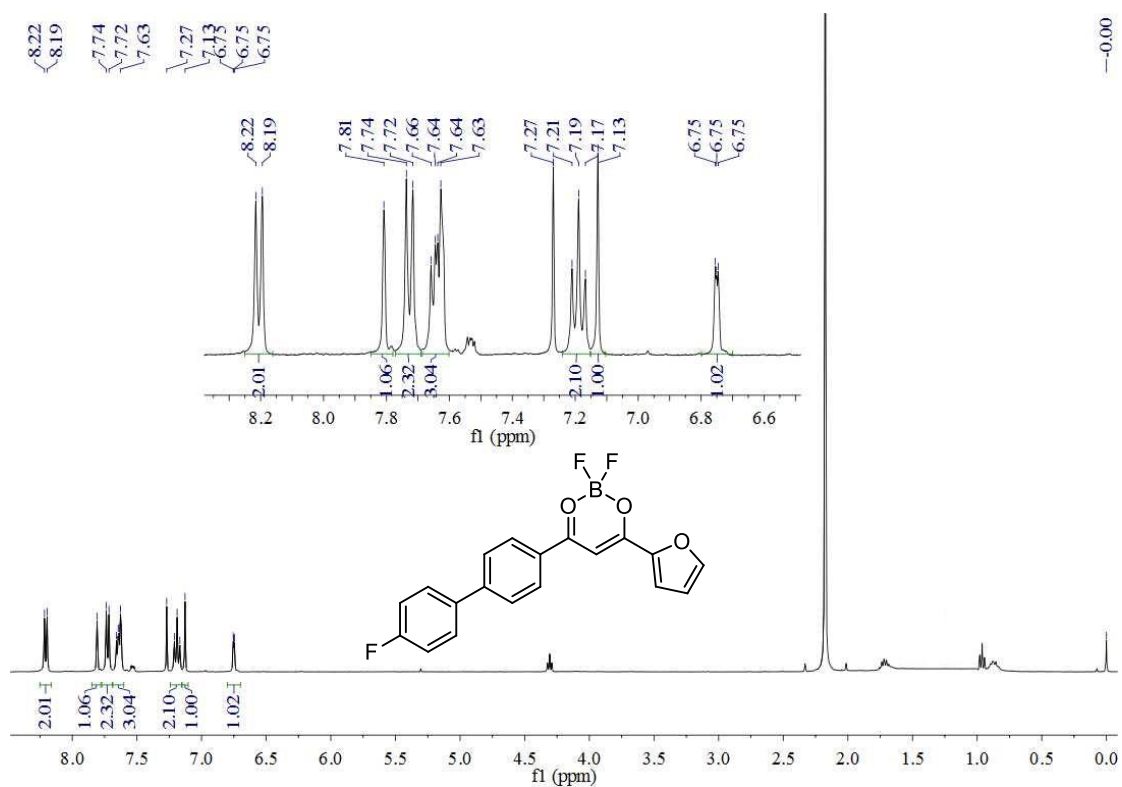


Figure S30. The ^1H NMR spectrum of complex F4 in CDCl_3 .

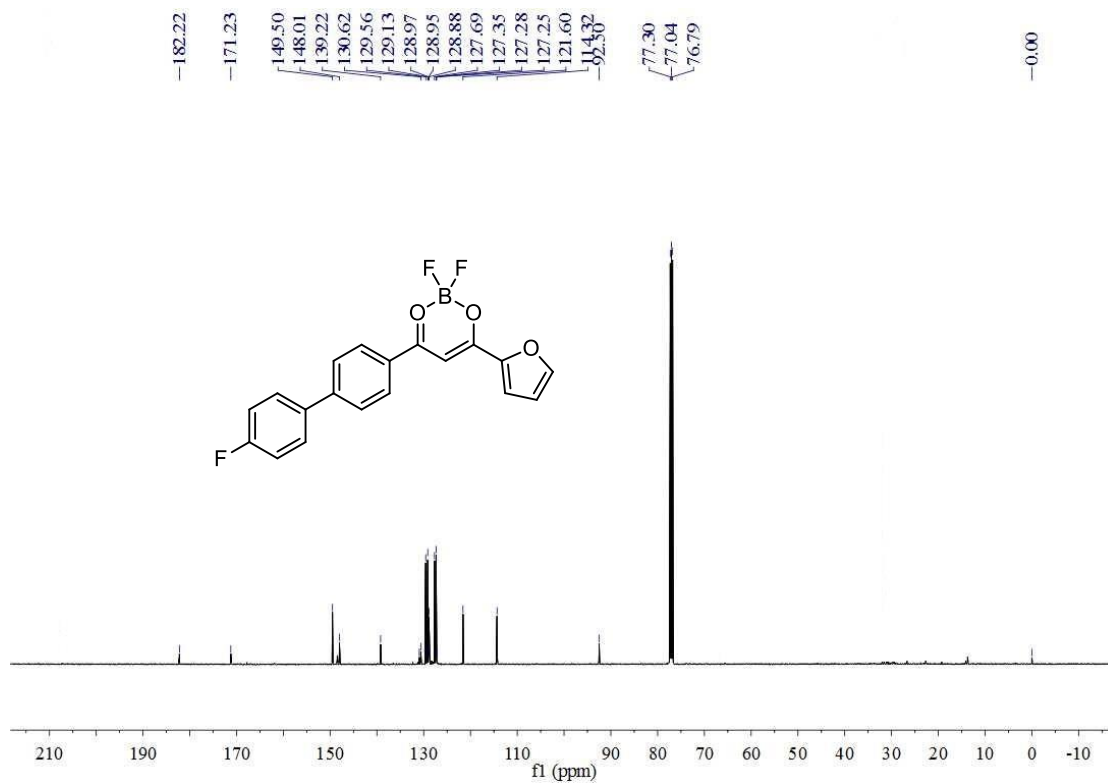


Figure S31. The ¹³C NMR spectrum of complex F4 in CDCl₃.

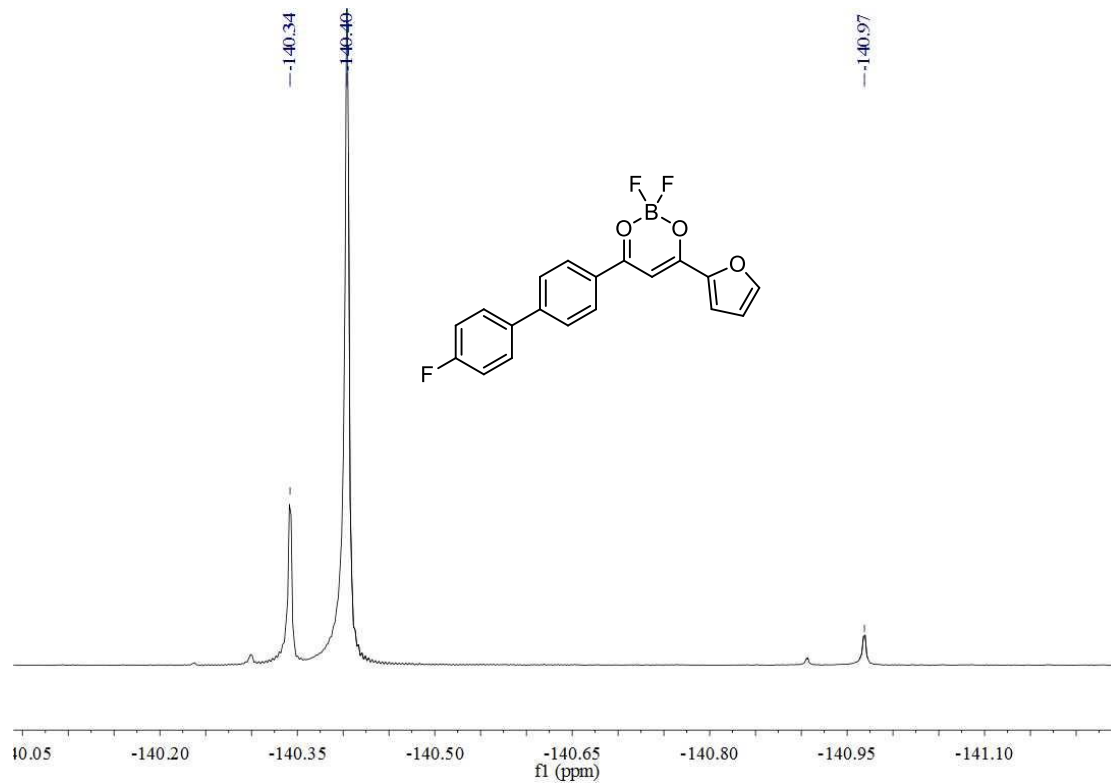


Figure S32. The ¹⁹F NMR spectrum of complex F4 in CDCl₃.

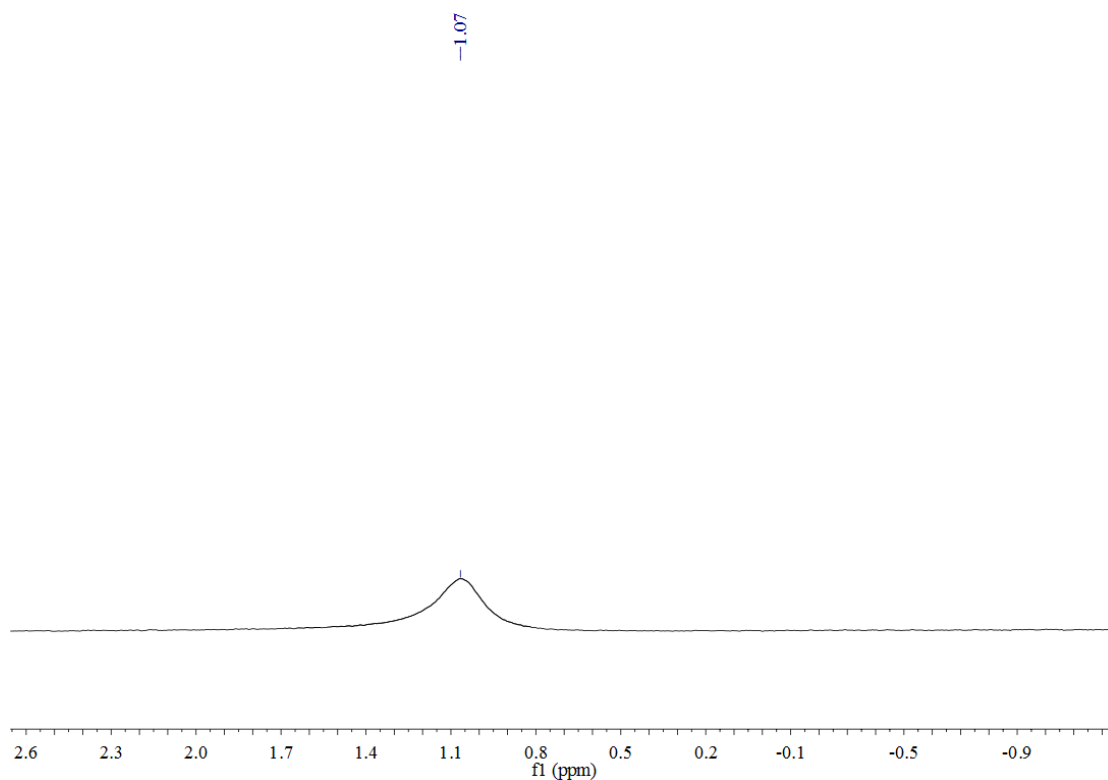


Figure S33. The ^{11}B NMR spectrum of complex F4 in CDCl_3 .

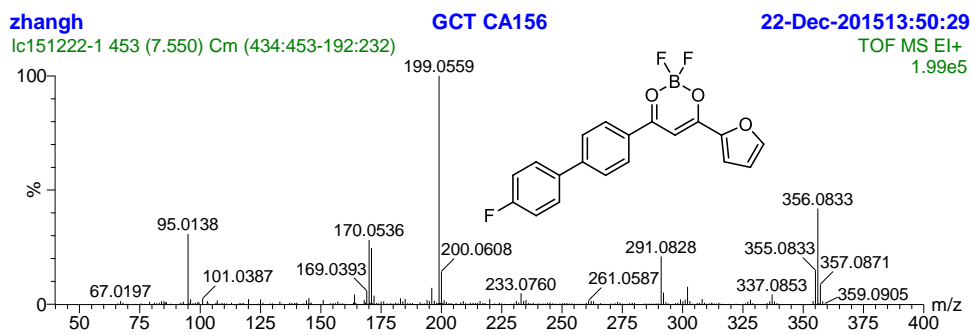


Figure S34. The HRMS spectrum of complex F4.

References

- [1] X. Jiang, X. Liu, Y. Jiang, Y. Quan, Y. Cheng and C. Zhu, *Macromol. Chem. Phys.*, 2014, **215**, 358-364.
- [2] G. Zhang, J. Chen, S. J. Payne, S. E. Kooi, J. Demas and C. L. Fraser, *J. Am. Chem. Soc.*, 2007, **129**, 8942-8943.