

Supplementary Information for Crystal

A Novel Phosphorescent Iridium(III) Complex Bearing Formamide for Quantitative Fluorine Anion Detection

Song Guo^{1,2}, *Chaoxiong Guo*², *Zhao Lu*², *Linlin Du*², *Man Gao*², *Shujuan Liu*¹, *Yuanli Liu*^{2,*} and *Qiang Zhao*^{1,*}

¹ State Key Laboratory of Organic Electronics and Information Displays & Jiangsu Key Laboratory for Biosensors, Institute of Advanced Materials, Nanjing University of Posts and Telecommunications, Nanjing 210023 Jiangsu, P. R. China; iamsguo@njupt.edu.cn (S. G.), iamsjliu@njupt.edu.cn (S. L.)

² Guangxi Key Laboratory of Optical and Electronic Materials and Devices, College of Materials Science and Engineering, Guilin University of Technology (GLUT), Guilin 541004, Guangxi, P. R. China; 1020190104@glut.edu.cn (C. G.), 1020190105@glut.edu.cn (Z. L.)

* Correspondence: lyuanli@glut.edu.cn (Y. L.), iamqzhao@njupt.edu.cn (Q. Z.)

Experimental Section

The chemical stability of complex 4: Seven copies of a solution of complex **4** in CH₂Cl₂ at the concentration of 1.0×10^{-5} M (2.0 mL) were prepared in a cuvette, then adding 0.5 mg solid powders of NaCl, NaBr, NaHCO₃, Na₂CO₃, CH₃COOK and Na₂SO₄ into six cuvettes, respectively (The molar ratio of the complex to the added anion was far less than 1:1). Next, the emission spectra of the seven samples were carried out, and the phosphorescent intensity at 535 nm was recorded as shown in Figure 3a (orange part). Then 0.5 mg tetrabutylammonium fluoride was added into the seven samples and the emission quenched immediately, the phosphorescent intensity at 535 nm was also recorded as shown in Figure 3a (gray part).

Fluoride Anion Detection: Preparing two solutions of complex **4** in CH₂Cl₂ (1.0×10^{-3} M, solution 1) and tetrabutylammonium fluoride (5.0×10^{-3} M, solution 2) in CH₂Cl₂ beforehand, respectively. Then, 0.2 mL solution 1 and different microliters of solution 2 (The specific value was shown in Figure S10) were added into a cuvette, and solvent CH₂Cl₂ was added into the cuvette until the total volume of the solution up to 2.0 mL. Then the emission spectrum of the mixture system was measured.

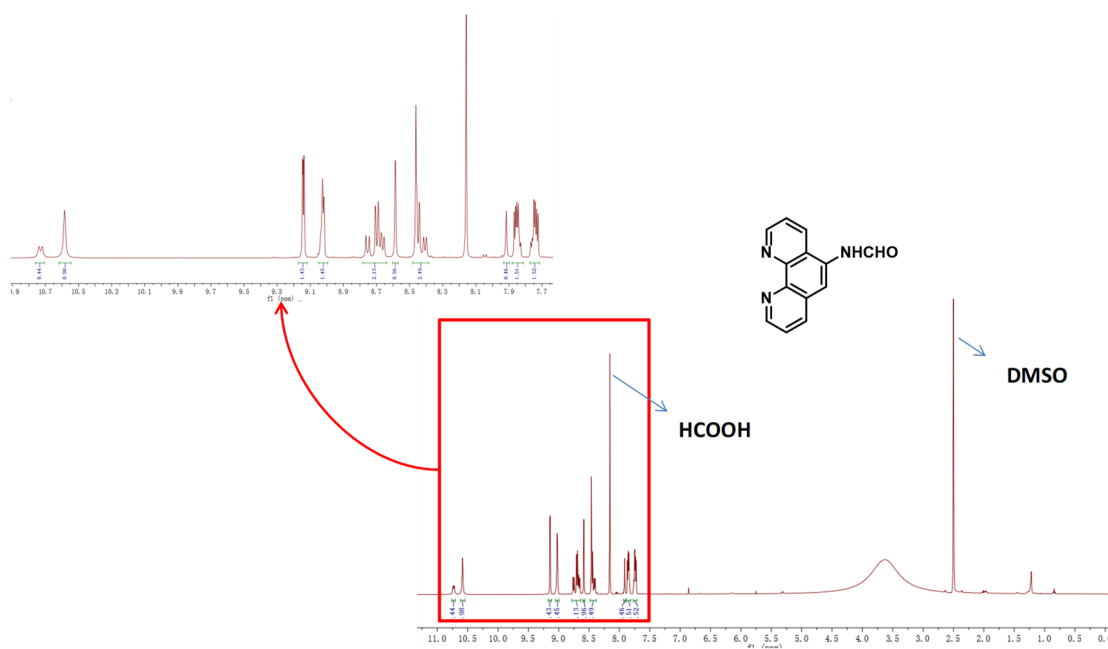


Figure S1. The ¹H spectrum of auxiliary ligand 2.

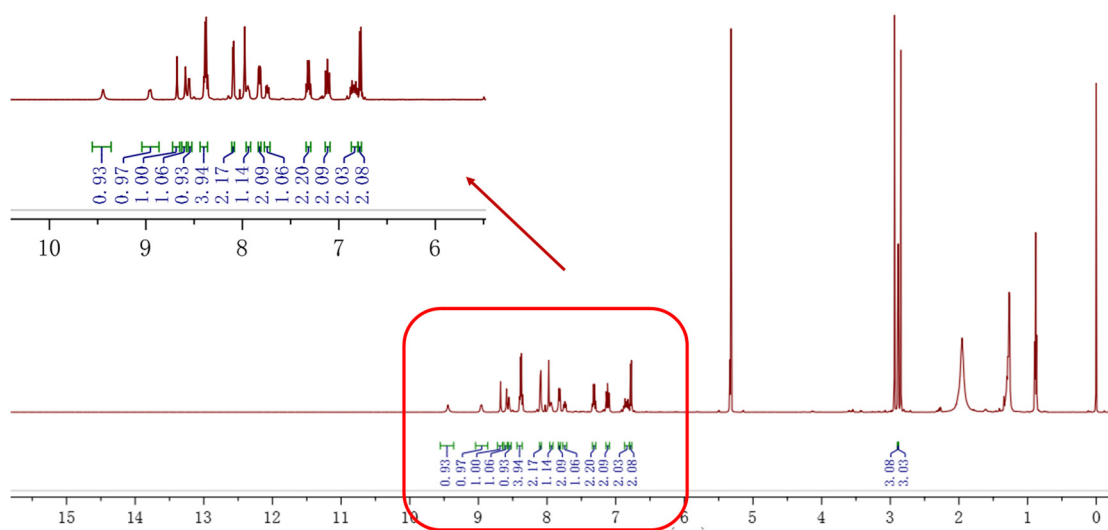


Figure S2. The ¹H spectrum of complex 4.

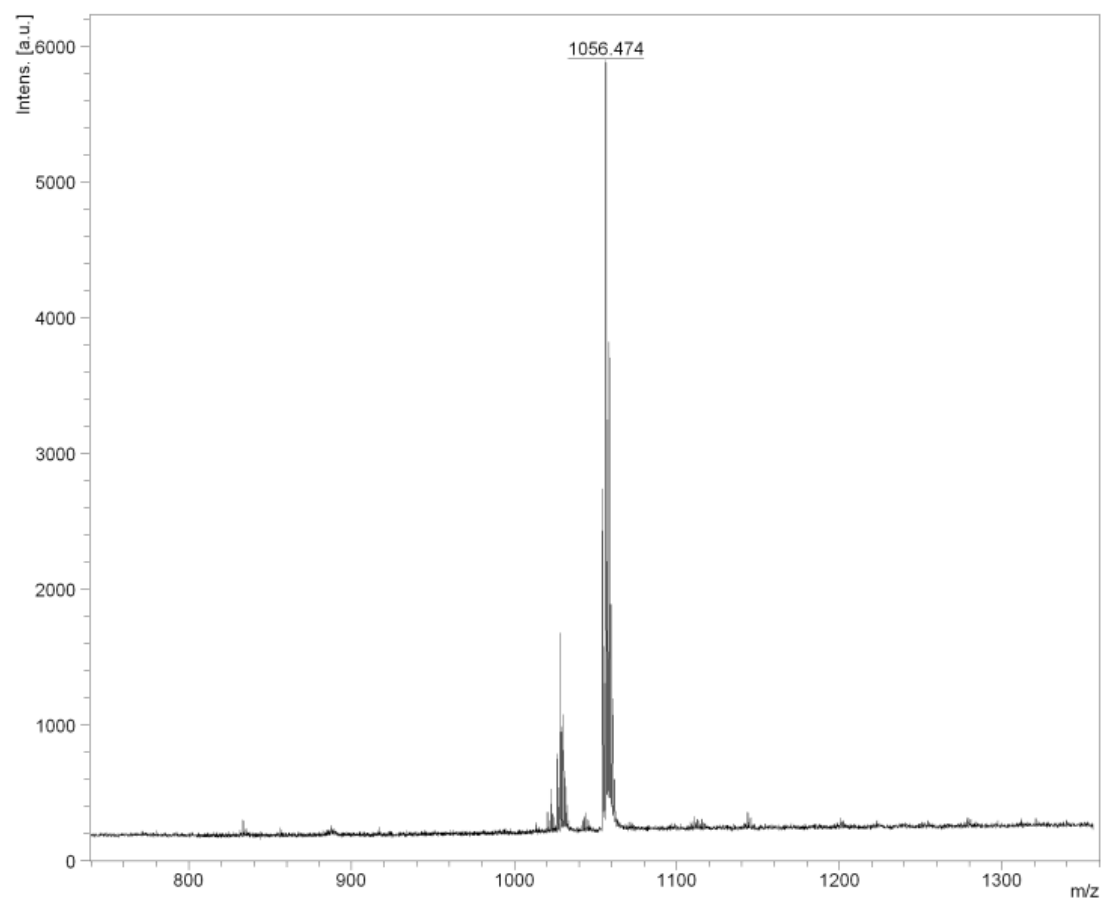


Figure S3. MALDI-TOF spectrum of complex **4**.

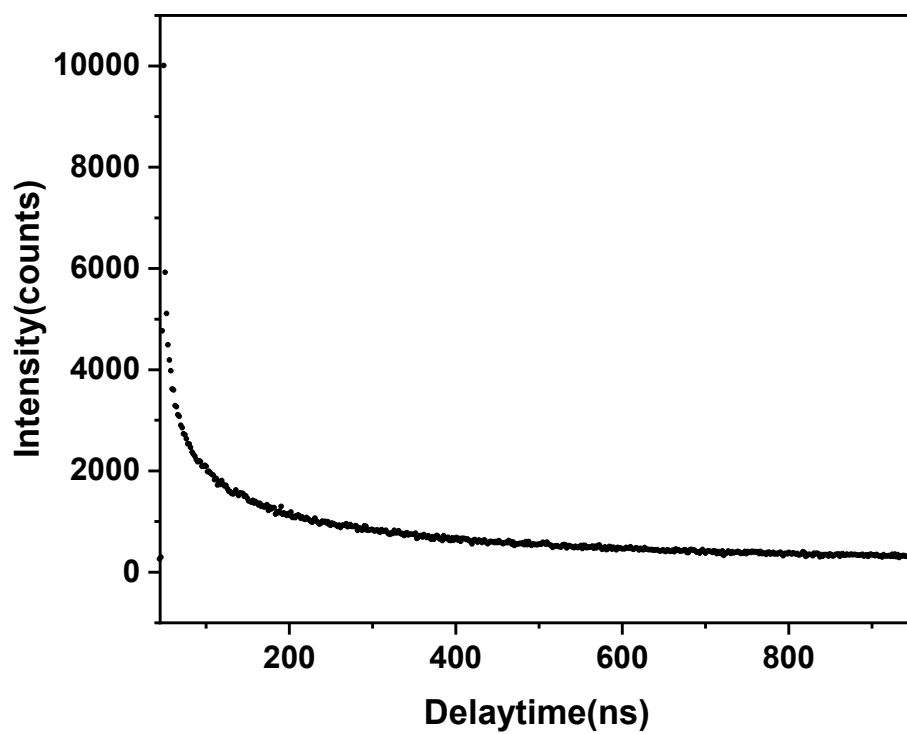


Figure S4. The decay curve of phosphorescent lifetime for complex 4 in solid state.

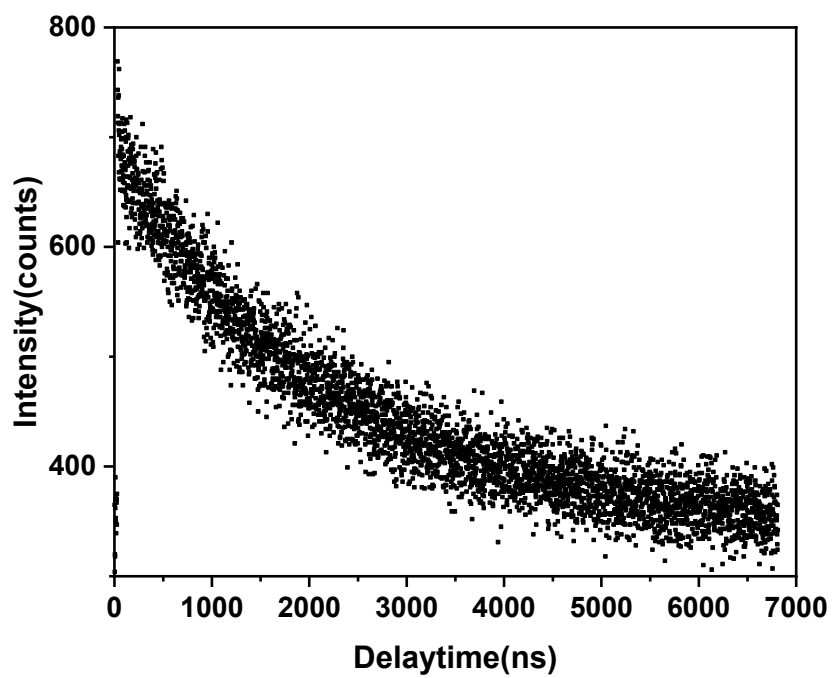


Figure S5. The decay curve of phosphorescent lifetime for complex 4 in CH_2Cl_2 .

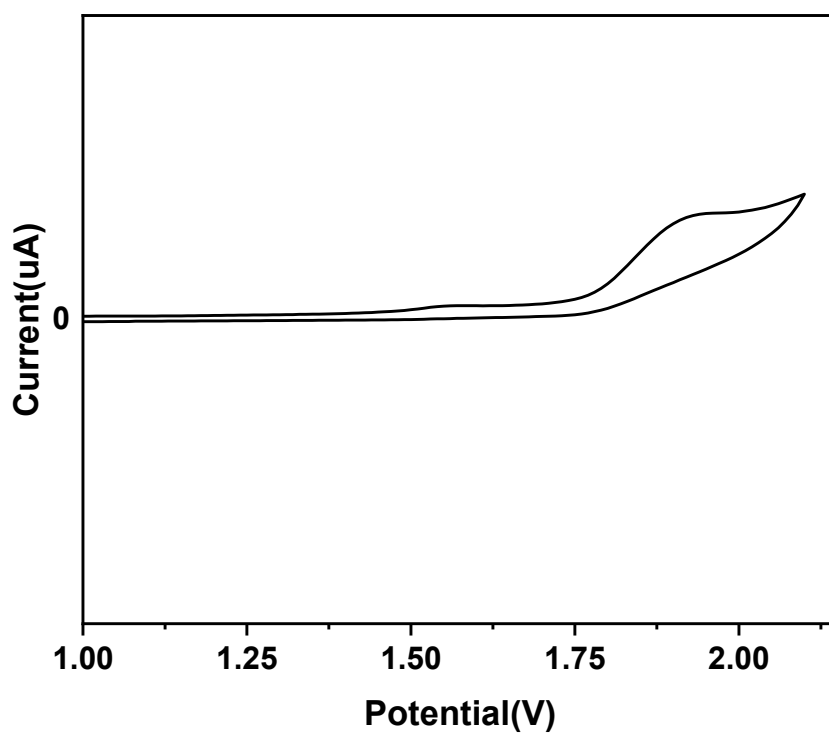


Figure S6. The cyclic voltammograms of **4** under a scan rate of 100 mV/s in CH₃CN.

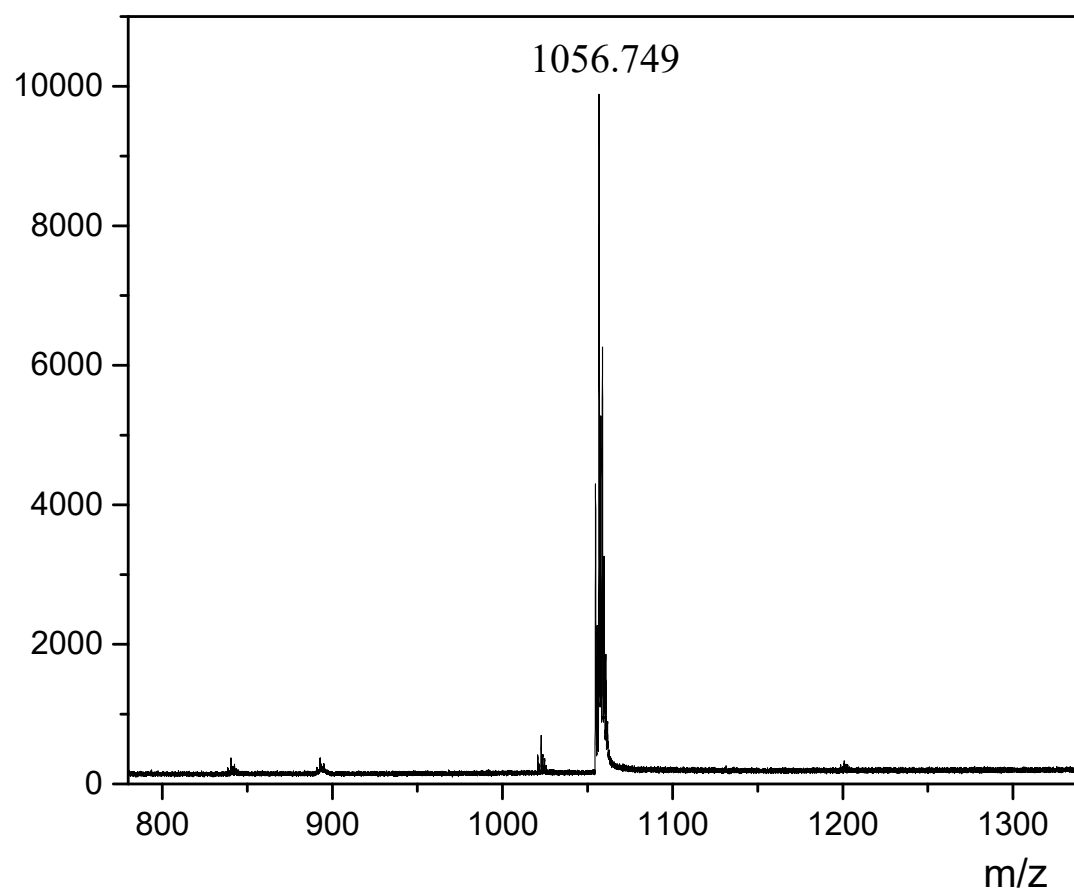


Figure S7. MALDI-TOF spectrum of complex **4** containing CO_3^{2-} .

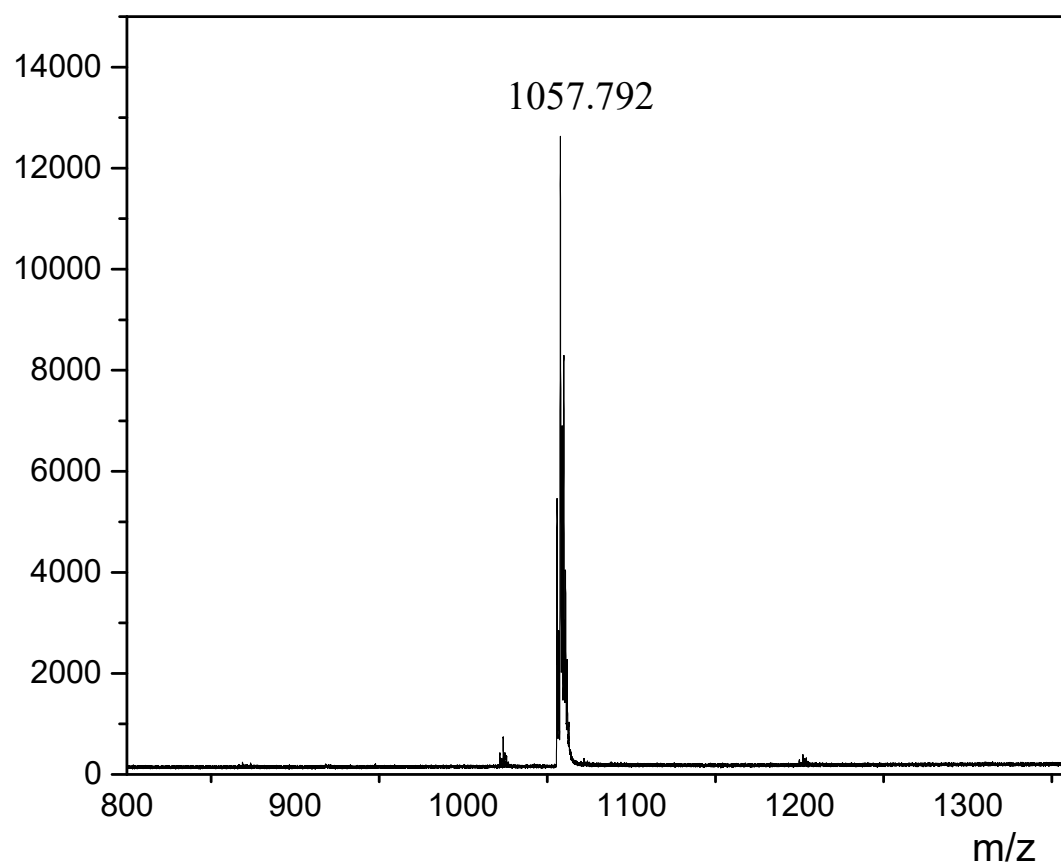


Figure S8. MALDI-TOF spectrum of complex **4** containing HCO_3^- .

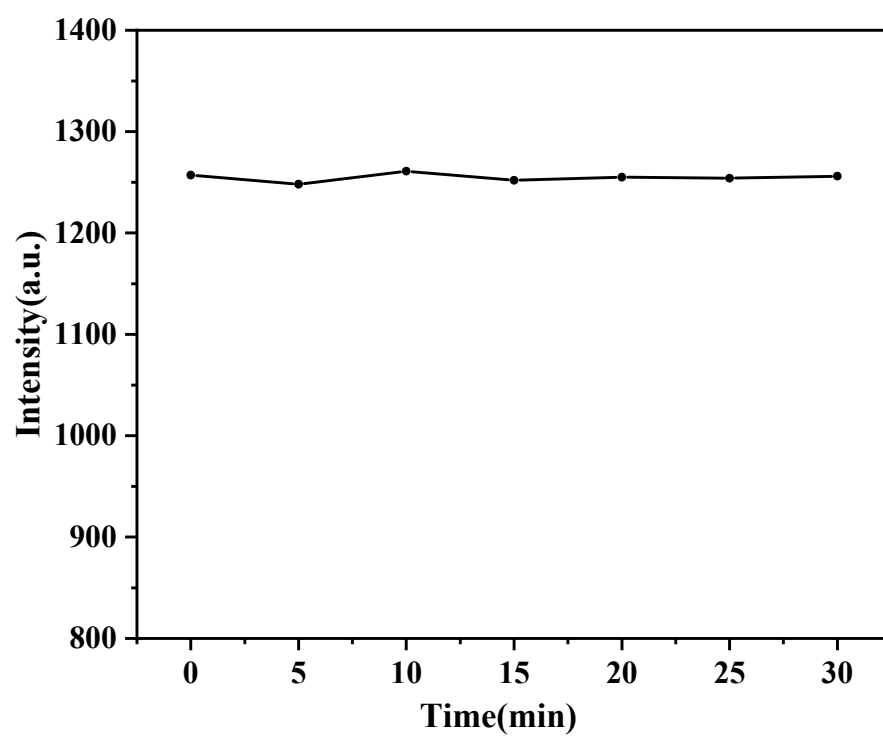


Figure S9. The photostability of complex **4** excited at 365 nm.

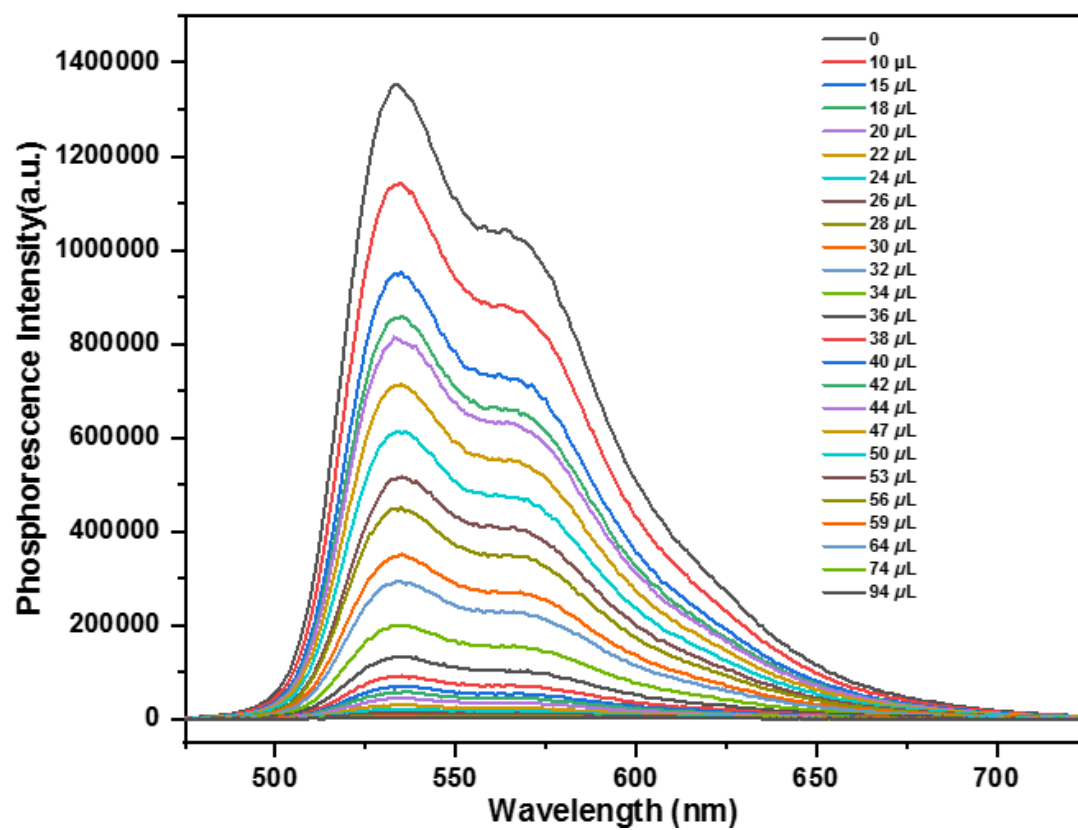


Figure S10. The emission spectra for the response of complex 4 to fluoride anion in dichloromethane.

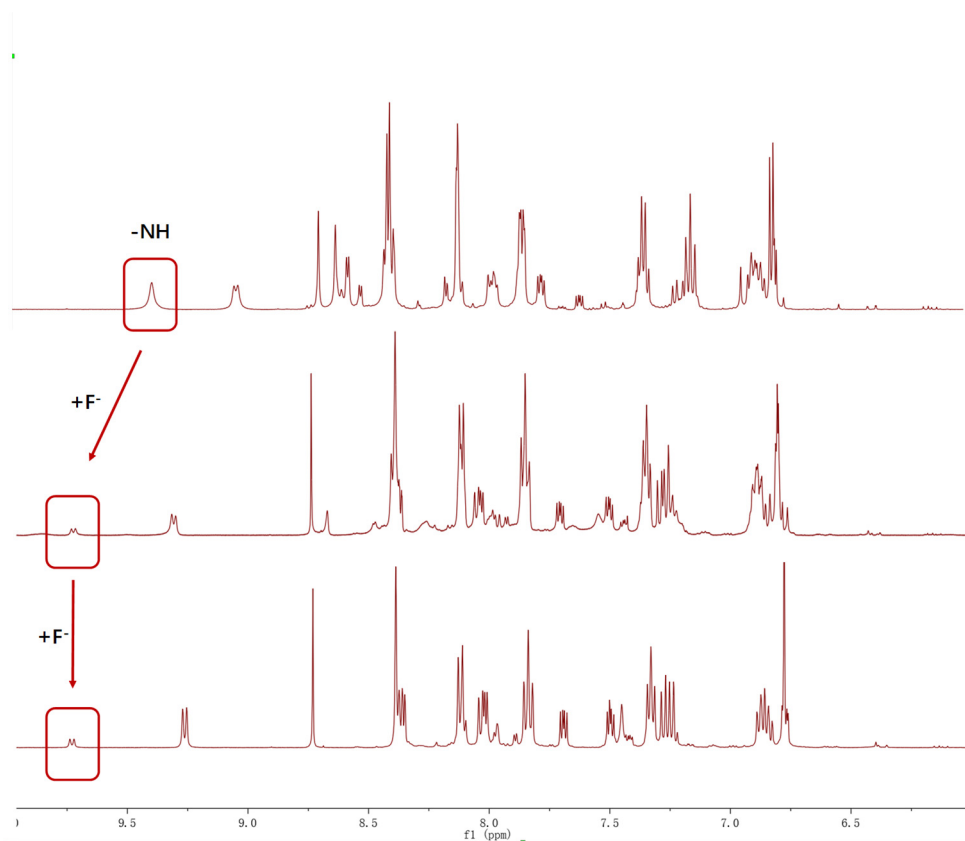


Figure S11. The ^1H NMR titration for complex **4**.

The upper spectrum was the solution of complex **4** in CD_2Cl_2 without F^- , the mid spectrum was the solution of complex **4** in CD_2Cl_2 containing 0.5 equivalent F^- , and the bottom spectrum was the solution of complex **4** in CD_2Cl_2 containing 1.0 equivalent F^- .

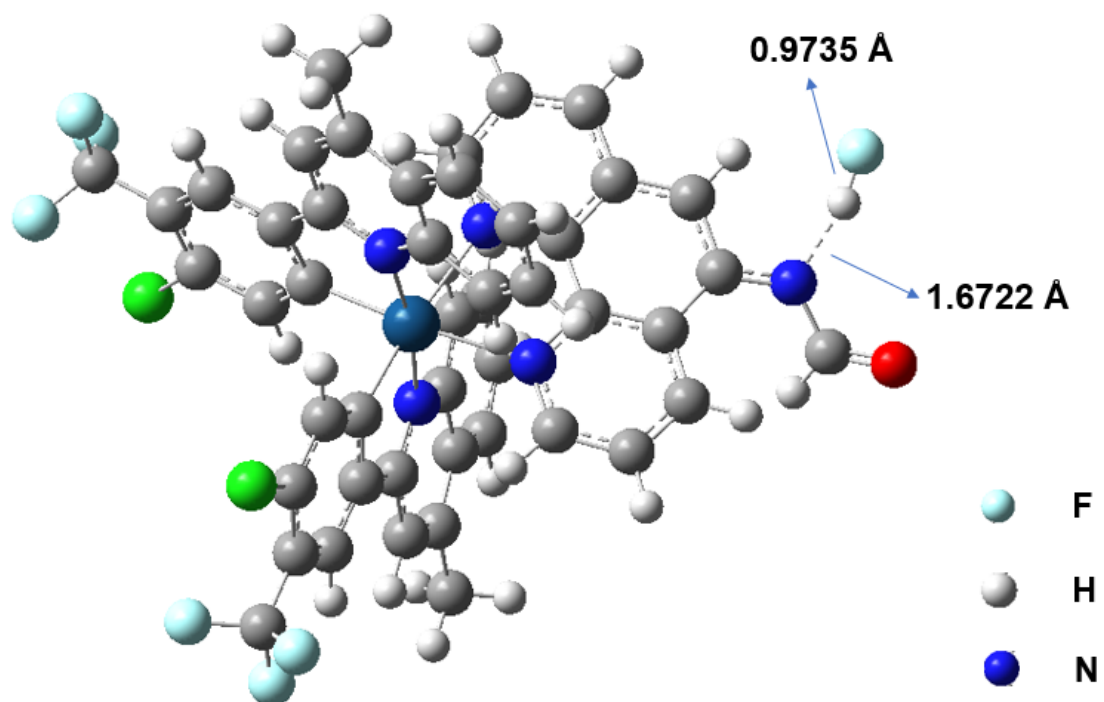


Figure S12. The molecular configuration of complex **4** with fluorine.

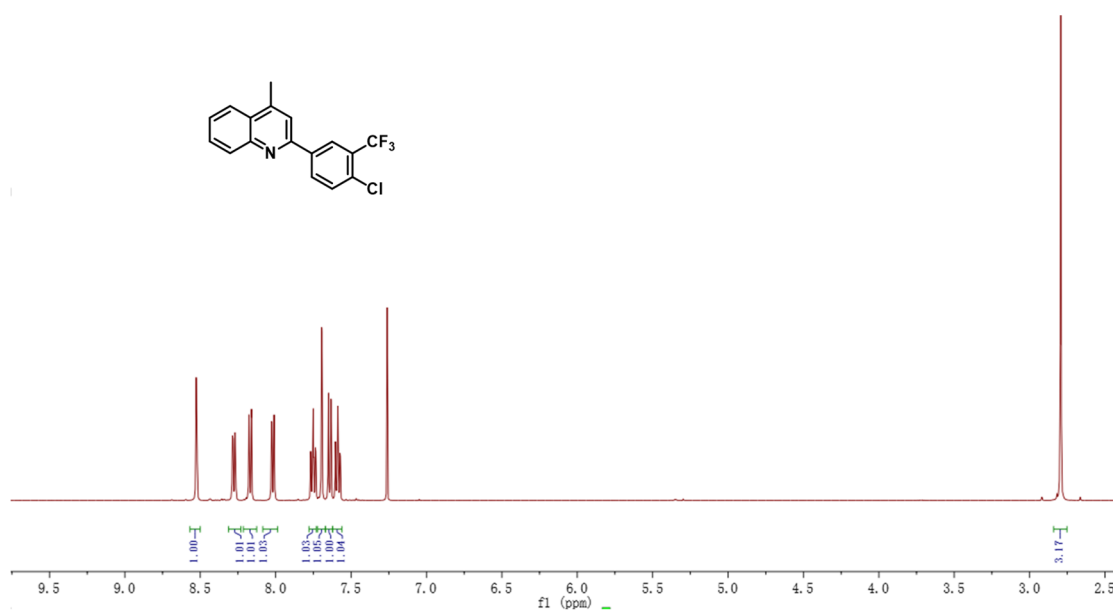


Figure S13. The ^1H spectrum of main ligand.

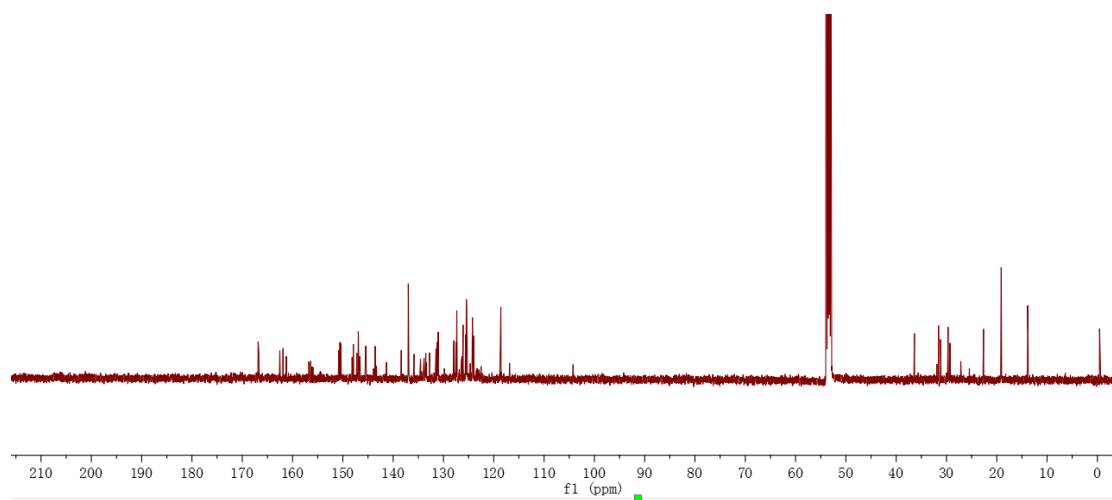


Figure S14. The ^{13}C spectrum of complex 4.

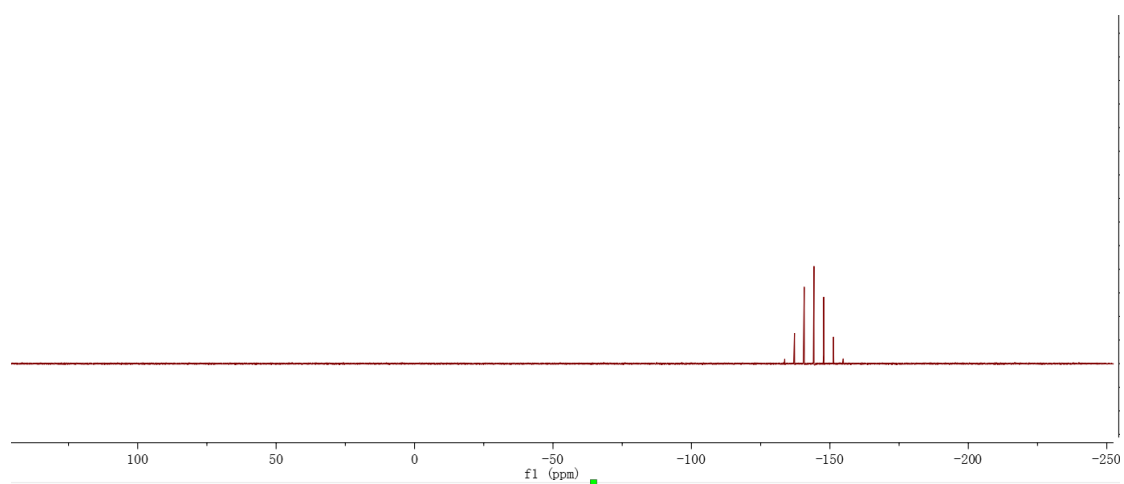


Figure S15. The ^{31}P spectrum of complex **4**.