

## Electronic Supplementary Information

# A multifunctional ionic iridium complex for field-effect and light-emitting device

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## Experimental section

*Synthesis of the ionic iridium light-emitting complex ([Ir(dmfpz)<sub>2</sub>(dtb-bpy)]PF<sub>6</sub>):* The ancillary ligand 4,4'-Bis(tert-butyl)-2,2'-bipyridine (dtb-bpy) was synthesized by a reported procedure.<sup>1</sup> The ligand 1-(9, 9-dimethyl-fluorene-2-yl)-1*H*-pyrazole (dmfpz) was synthesized by the following routes. Firstly, 60 mL dimethyl sulfoxide was added into fluorene (10 g, 60 mmol) under an argon atmosphere for 1.5 hours, and then iodomethane (9.35 mL, 150 mmol) was added into the reaction mixture under stirring, resulting in a suspension. After filtration, the solution was rotary evaporated to get a yellow product (9.78 g, 50.91 mmol). Secondly, the yellow product (7.90 g, 40 mmol) was added into a boiling mixed solution (67 wt.% acetic acid, 27 wt.% deionized water and 2 wt.% vitriol). Periodic acid (1.57 g, 6.89 mmol) and iodine (3.40 g, 13.39 mmol) were then added into the cooled mixture (60 °C). After stirring for 4 hours, the precipitate was washed with Na<sub>2</sub>CO<sub>3</sub> saturated aqueous solution. A kind of light yellow grease (10.15 g, 31.80 mmol) was got after recrystallization. Thirdly, dodecane (4.41 g, 26 mmol), the light yellow grease (10.15 g, 31.72 mmol), trans-cyclohexanediamine (0.26 mL, 2.28 mmol) and 30 mL 1,4-epoxy hexane were successively added into a mixture of CuI (0.22 g, 1.15 mmol), pyrazole (1.76 g, 26.07 mmol) and K<sub>2</sub>CO<sub>3</sub> (6.3g, 46 mmol) under an argon atmosphere. The mixture was stirred at 110 °C for 24h and then cooled to get an oily product. The crude product was washed with CH<sub>2</sub>Cl<sub>2</sub> and purified by column chromatography on silica gel (200-300 mesh) with petroleum ether/CH<sub>2</sub>Cl<sub>2</sub> (2:1) to get the ligand 1-(9, 9-dimethyl-fluorene-2-yl)-1*H*-pyrazole (dmfpz). The dichloro-bridged diiridium

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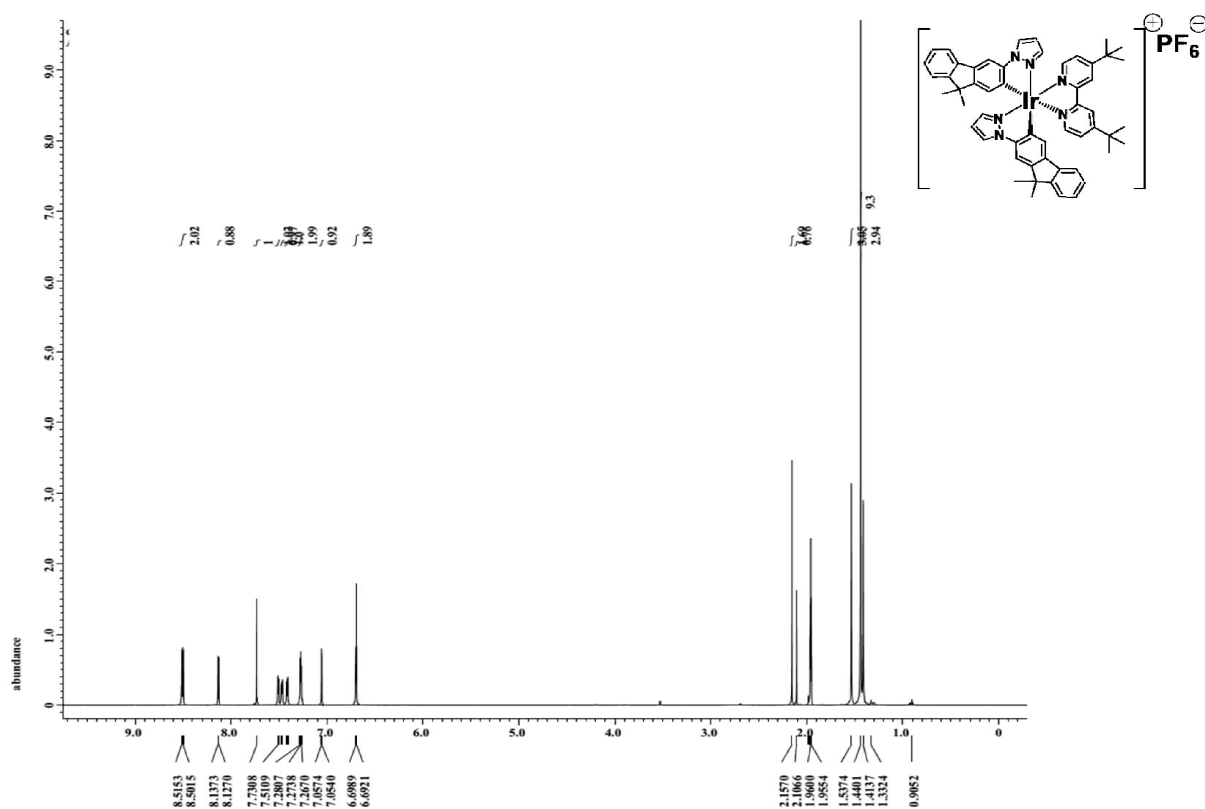
complex  $[\text{Ir}(\text{dmfpz})_2\text{Cl}]_2$  and the ancillary ligand, dtb-bpy were dissolved in 1,2-ethanediol and refluxed at 150 °C for 15 h under an argon atmosphere. The reaction mixture was then cooled to room temperature, followed by the adding of a aqueous solution of  $\text{NH}_4\text{PF}_6$  (3.0 g in 15 mL deionized water) under stirring. After filtrated, the precipitate was washed with deionized water and methanol, and dried under vacuum at 60°C for 12h. The crude product was then purified by column chromatography on silica gel (200-300 mesh) with  $\text{CH}_2\text{Cl}_2/\text{acetone}(50:1)$ , yielding a yellow powder (1.15g, 1.17 mmol). Yield: 87%.  $^1\text{H}$  NMR (600 MHz, acetone- $d_3$ ,  $\delta$ ): 8.50 (dd,  $J = 8.16$  and  $2.76$  Hz, 4H), 8.13 (d,  $J = 6.18$  Hz, 2H), 7.73 (s, 2H), 7.51-7.41 (m, 4H), 7.28-7.27 (m, 4H), 7.05 (d,  $J = 2.04$  Hz, 2H), 6.70 (t,  $J = 4.08$  Hz, 4H), 1.54 (s, 6H), 1.44(s, 18H), 1.41(s, 6H). MS (ESI) [ $m/z$ ]: 979.40 ( $M\text{-PF}_6$ )<sup>+</sup>. Anal.calcd for  $\text{C}_{54}\text{H}_{54}\text{F}_6\text{IrN}_6\text{P}$ : C, 57.69; H, 4.84; N, 7.48. Found: C, 56.77; H, 4.72; N, 7.53.

*Photo physical and electrochemical measurements:* Absorption spectra were performed with a UV-vis spectrophotometer (Agilent 8453). PL spectra were recorded by a fluorospectro-photometer (JobinYvon, FluoroMax-3). A Princeton Applied Research potentiostat/galvanostat model 283 voltammetric analyzer was used to collect cyclic voltammetry curves.

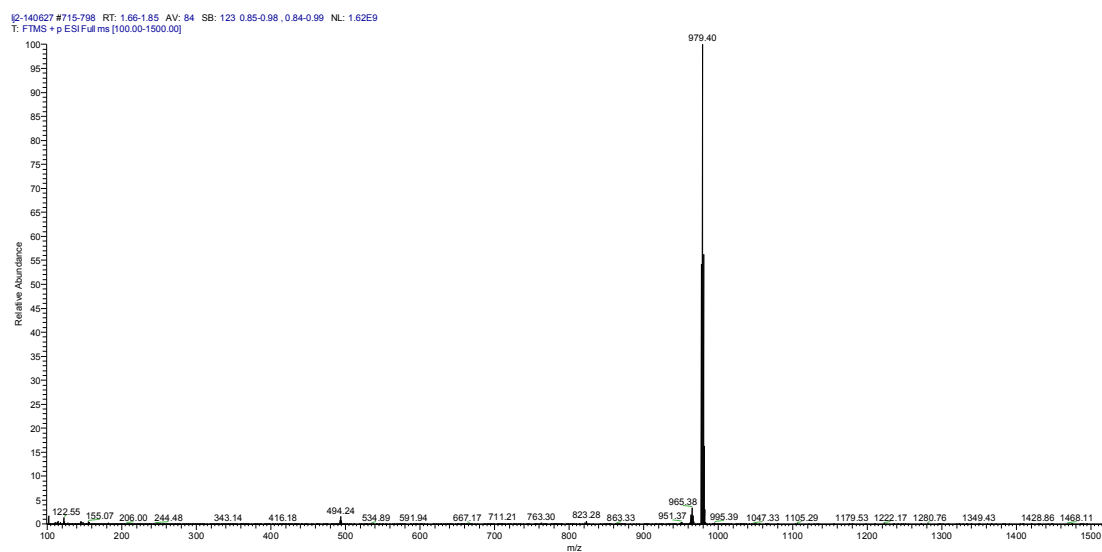
*Device Fabrication:* Glass substrate with ITO source and drain electrodes patterned on it (the channel width and length are 1000  $\mu\text{m}$  and 30  $\mu\text{m}$ ) was cleaned and treated with oxygen plasma before use. A ZTO layer (40 nm) was formed on the substrate by

the way published,<sup>2</sup> and then the ionic iridium complex (25 mg/mL in CH<sub>2</sub>Cl<sub>2</sub>) layer (100 nm) was spin-coated at 1500 rpm and baked at 80°C for 20 minutes. Device was then transferred into a metal evaporating chamber where an Ag cathode (80 nm) was evaporated at an evaporating rate of 0.5~1 Å s<sup>-1</sup>.

*Electrical and electroluminescent measurements:* Measurements were carried out in ambient conditions. We used Keithley4200 semiconductor characterization systems to measure the electrical properties. And a Photo Research PR705 spectro-photometer was used to collect the electroluminescent spectrum.



**Figure S1.** <sup>1</sup>H NMR spectrum of [Ir(dmfpz)<sub>2</sub>(dtbbpy)]PF<sub>6</sub> (acetone-d<sub>3</sub>).



**Figure S2.** Mass spectrum of  $[\text{Ir}(\text{dmfpz})_2(\text{dtb-bpy})]\text{PF}_6$  (acetonitrile).

References:

- (1) D. J. Awad, A. Koch, W. Mickler, U. Schilde and P. Z. Strauch, *Anorg. Allg. Chem.* 2012, **638**, 965.
- (2) Y. Zhao, L. Duan, G. Dong, D. Zhang, J. Qiao, L. Wang and Y. Qiu, *Langmuir* 2013, **29**, 151.