Supplementary material (ESI) for Journal of Materials Chemistry

Supporting Information

Procedure for the synthesis of Ir(MPCPPZ)$_3$ and the fabrication of PLEDS devices:

HMPCPPZ was easily synthesized via a nucleophilic substitution reaction between 1-chloro-4-(4-chlorophenyl) phthalazine (2.75 g, 10 mmol) and 2, 6-dimethylphenol (1.22 g, 10 mmol), using potassium carbonate (2.76 g, 20 mmol) in N, N'-dimethylformamide (10 mL). The iridium complex was directly synthesized from the obtained free ligand (1.44g, 4mmol) and $IrCl_3 \cdot 3H_2O$ (0.35 g, 1mmol) in the degassed mixed solution of 2-ethoxyethanol (15mL) and water (5mL). The temperature was maintained at 80 °*C* for 12 *h*. After cooling to room temperature, the solution filtered and the orange solid was washed with ethanol. Then the iridium complex was obtained after Al_2O_3 column purification with hexane/dichloromethane eluent. A single crystal suitable for X-ray diffraction was obtained from a mixed solution of hexane and dichloromethane.

The layer thickness was monitored upon deposition by using a crystal thickness monitor (Sycon). Device fabrication was carried out in a controlled atmosphere dry-box (Vacuum Atmosphere Co.) under N_2 circulation. Current density(J)-voltage(V)-luminance(L) data were collected using a keithley 236 source measurement unit and a calibrated silicon photodiode. Absolute PL efficiencies were measured in an integrating sphere (IS-080, Labsphere) under excitation from the 325 nm line of a HeCd laser. External EL quantum efficiencies were obtained by measuring the total light output in all directions in an integrating sphere (IS-080, Labsphere). The luminance and luminous efficiency were measured by a silicon photodiode and calibrated using a PR-705 SpectraScan Spectrophotometer (Photo Research). Photoluminescence spectra and electroluminescence spectra were recorded using a CCD spectrophotometer (Instaspec 4, Oriel). PL efficiency and PLspectra were taken under the 325 nm line of a HeCd laser and with 350 nm filter.

Spectroscopic and Elemental Analysis:

^{1}H NMR (400 MHz, $DCCl_3$, δ): 8.84(s, 2H), 8.82(s, 2H), 8.28(d, J=1Hz, 2H), 8.26(d, J=1Hz, 2H), 8.00(s, 2H), 77.97(s, 3H), 7.94-7.97(m, 3H), 7.85-7.89(m, 3H), 6.86(d, J=6Hz, 2H), 6.85(d, J=7Hz, 2H), 6.70(d, J=7Hz, 4H), 5.92-5.95(m, 3H), 2.16(s, 18H). ^{13}C NMR (400 MHz, $CDCl_3$, δ): 30.66, 119.55, 119.64, 123.55, 123.82, 125.65, 129.02, 129.06, 130.80, 131.98, 134.86, 136.00, 142.20, 149.80, 157.13, 158.94, 166.50, 206.87. Fast atom bombardment mass spectroscopy (FABMS): Calcd for $C_{66}H_{48}Cl_3N_6O_3Ir$, 1271.7, m/e=1272.0 (M^++1). Anal. calcd for $C_{66}H_{48}Cl_3N_6O_3Ir$: C 62.34, H 3.80, N 6.61, Cl 8.36; found: C 62.14, H 3.85, N 6.55, Cl 8.30.

[CCDC 670325 contains 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.]

List of Figures

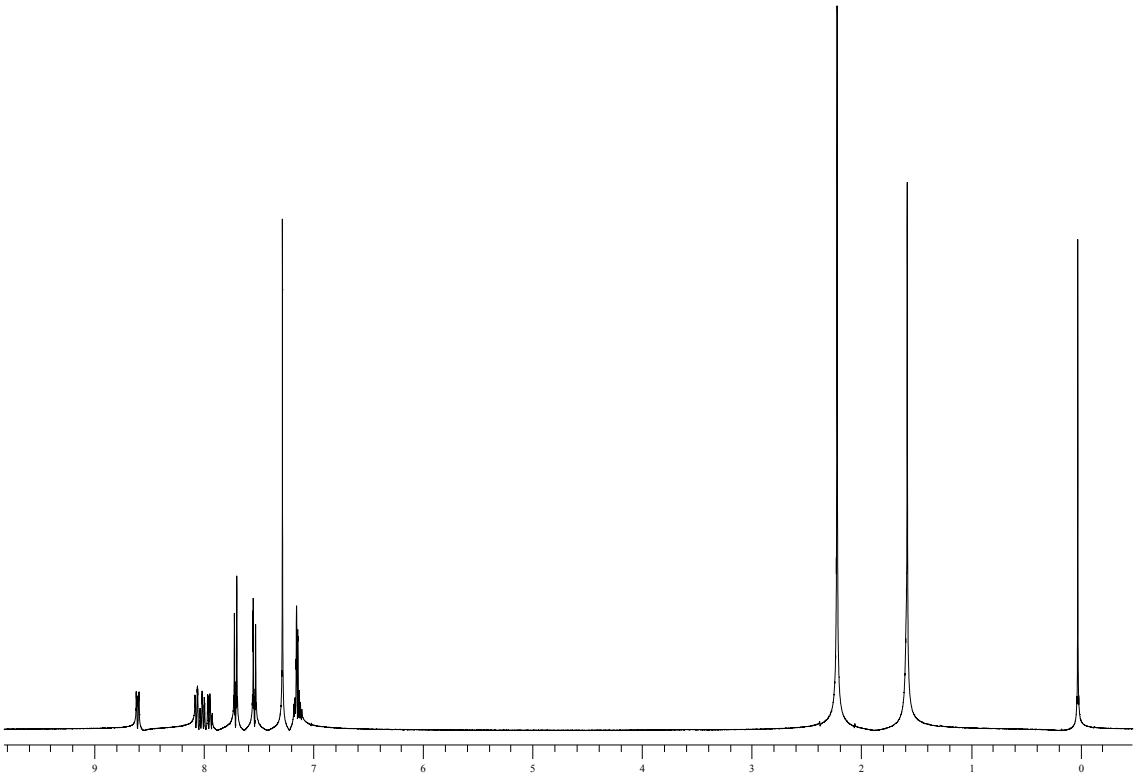

Fig 1 ^{1}H NMR (400 MHz, $DCCl_3$, δ) of HMPCPPZ.

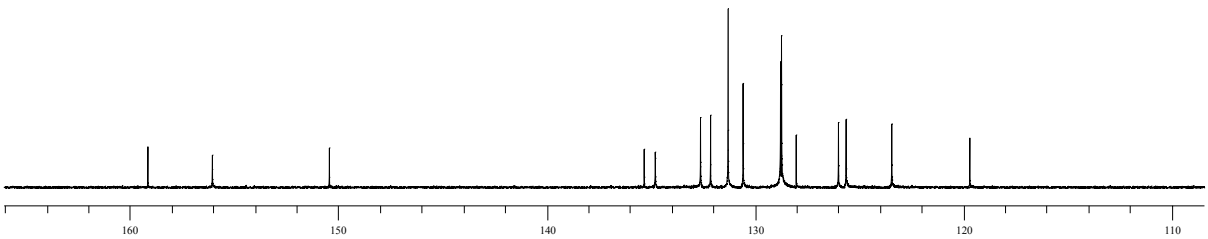

Fig 2 ^{13}C NMR (400 MHz, $DCCl_3$, δ) of HMPCPPZ.

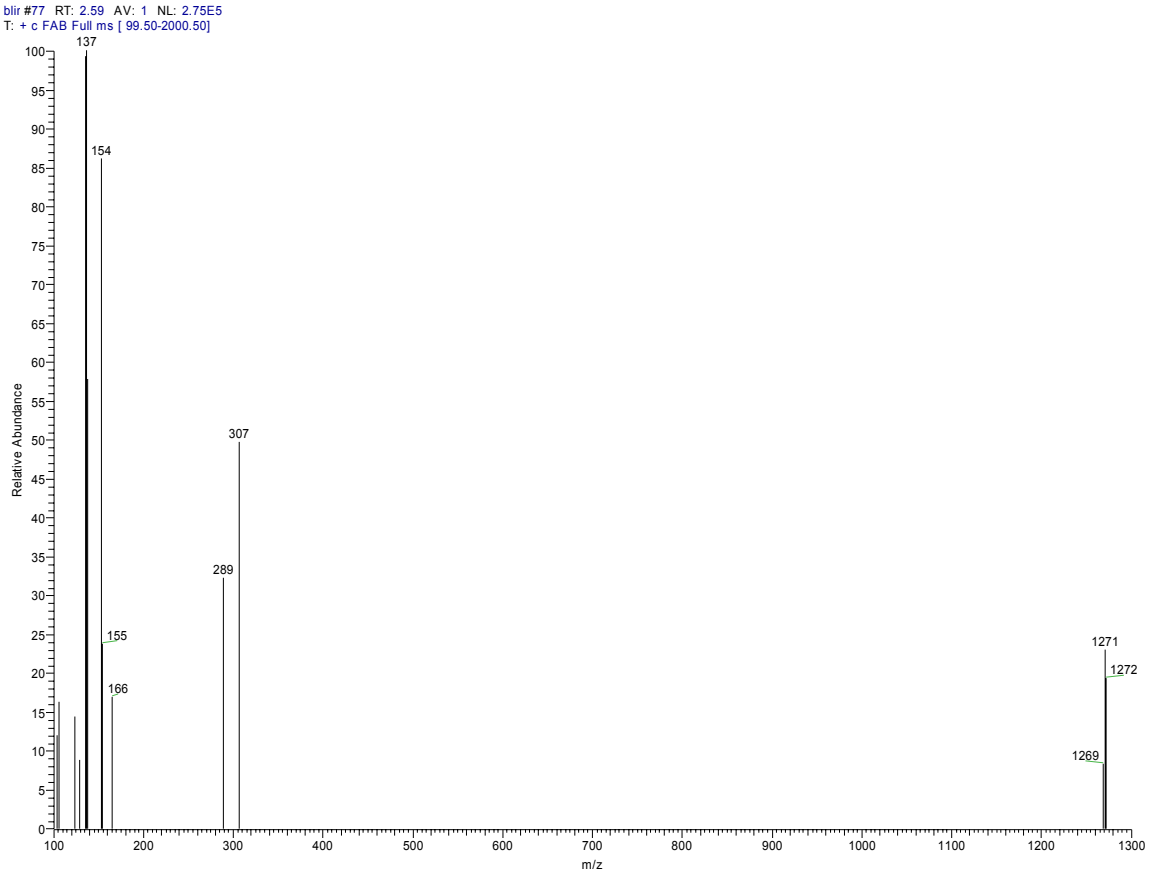

Fig 3 The FABMS of $Ir(MPCPPZ)_3$.

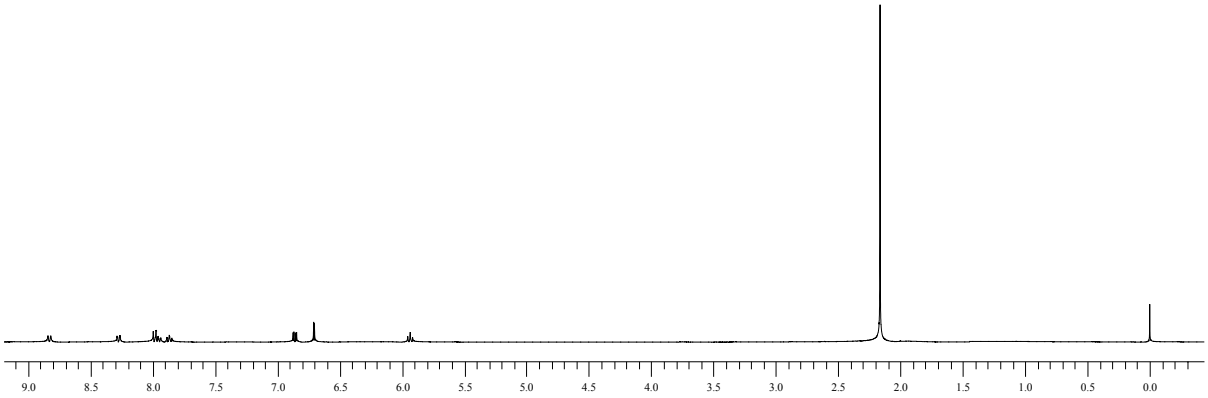

Fig 4 ^{1}H NMR (400 MHz, $DCCl_3$, δ) of $Ir(MPCPPZ)_3$.

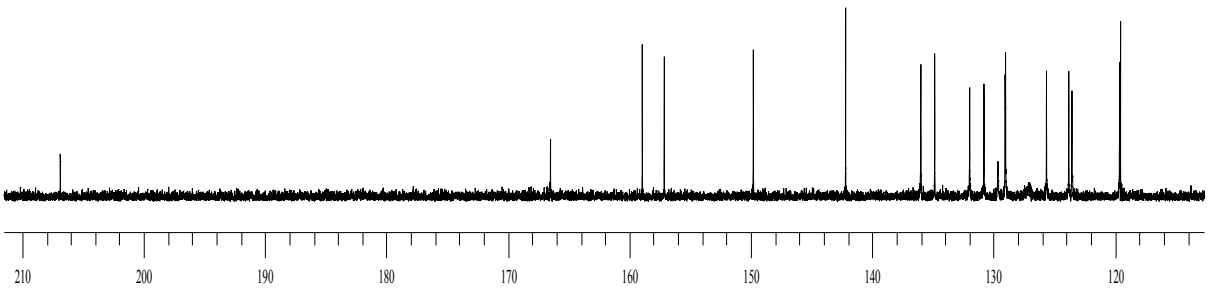

Fig 5 ^{13}C NMR (400 MHz, $DCCl_3$, δ) of $Ir(MPCPPZ)_3$.

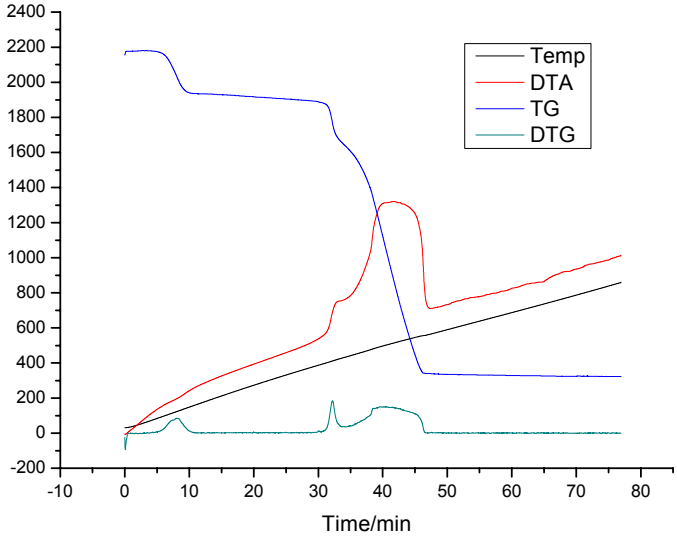

Fig 6 The thermogravimetric analysis of $Ir(MPCPPZ)_3$.

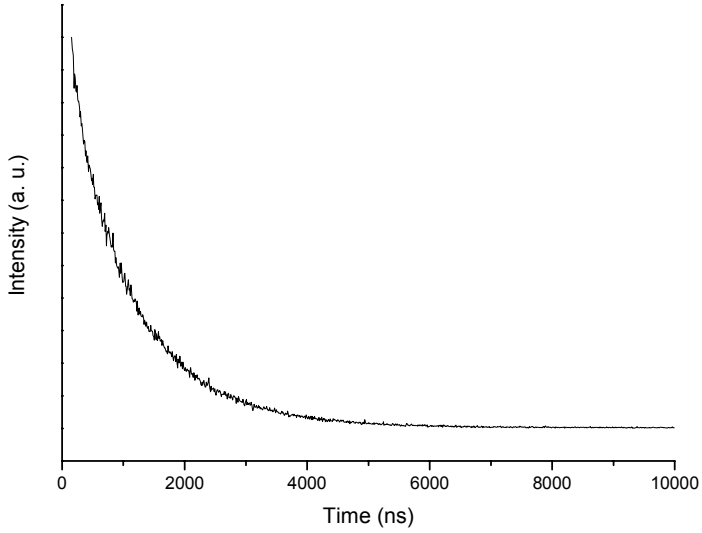

Fig 7 The decay curve of $Ir(MPCPPZ)_3$ in solid film excited at 468 nm.

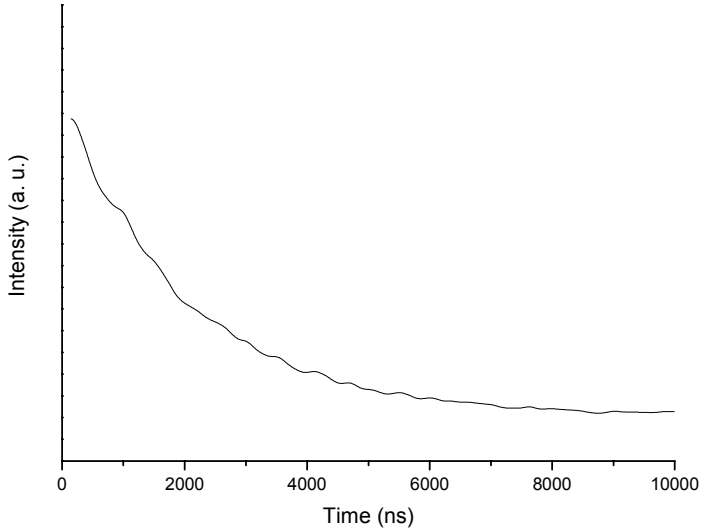

Fig 8 The decay curve of $Ir(MPCPPZ)_3$ in degassed CH_2Cl_2 excited at 468 nm.