

## Supporting Information

Figure.S1. Cyclic voltammograms of complex 2-4 and Na[BPh<sub>4</sub>].

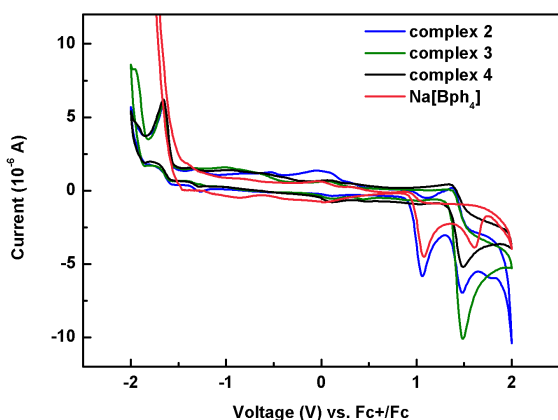
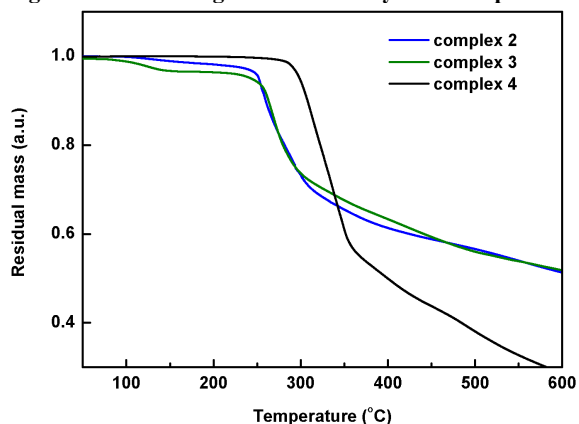
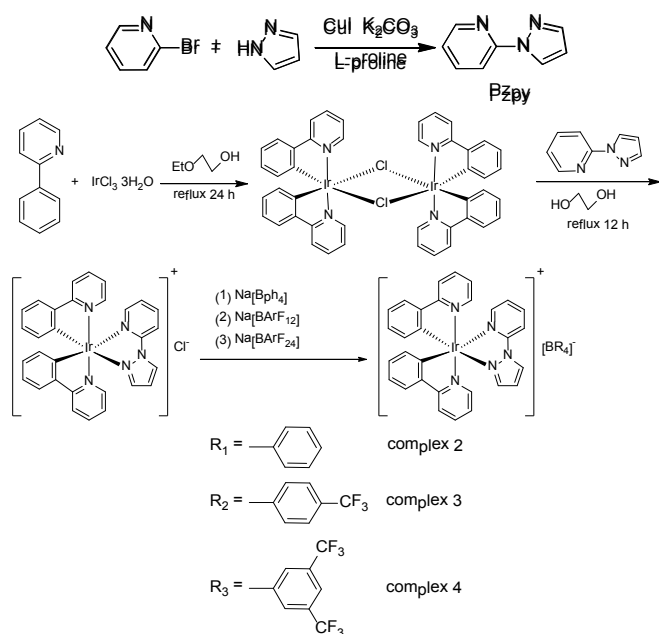


Figure.S2. Thermal gravimetric analysis of complex 2-4.



Scheme.S1. Synthetic routes of complexes 2-4.



## Notes and references

**Crystal Data:** Crystallographic data of complex 1-3 can be found in CCDC680949, CCDC963326 and CCDC963327, which can be obtained free of charge from the Cambridge Crystallographic Data Centre from [www.ccdc.cam.ac.uk/conts/retrieving.html](http://www.ccdc.cam.ac.uk/conts/retrieving.html).

**Quantum chemical calculations:** Calculations on the ground states of complexes 1-4 were carried out using density functional theory (DFT) at the B3LYP level<sup>[1,2]</sup>, with the X-ray single-crystal structures. The basis sets employed for the C, H, N, and F were 6-31G\*. All the calculations were performed with Gaussian 09 software package with a spin-restricted formalism<sup>[3]</sup>.

- 1 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648.
- 2 C. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B.*, 1988, **37**, 785.
- 3 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09*, Revision A.02; Gaussian, Inc., Wallingford CT, 2009.