

D-2-2

Efficient Red Electrophosphorescent Devices Based on Iridium Complexes of Fluorinated 1-phenylisoquinoline

Gui Youn Park^{1*}, Ji-hyun Seo¹, Dong-il Yoo², Young Kwan Kim³,
Young Sik Kim³ and Yunkyoung Ha³

¹Department of Information Display Engineering, Hongik University, Seoul 121-791, Korea

²Department of Chemical Engineering, Hongik University

³Department of Science, Hongik University, Seoul, 121-791, Korea

Phone: +82-2-320-1490 , E-mail: ykha@hongik.ac.kr

1. Introduction

Organic light-emitting devices (OLEDs) have been extensively studied for application in flat-panel displays due to rapid progress in material design and device fabrication in recent years. OLEDs based on phosphorescent materials can significantly improve electroluminescence performance because both singlet and triplet excitons can be harvested for light emission. However, most of phosphorescent emitters have a long lifetime which results in saturation of emissive sites at increasing currents. It leads to dominant triplet-triplet annihilation at high currents and the maximum external quantum efficiency is lower than 2%.

Recently, the Ir(III) complexes having the relatively short phosphorescent lifetime has been reported. Ir(piq)₂(acac) has been a known red phosphorescent emitter, which exhibits an emission peak at 622 nm, the external EL quantum efficiency of 8.46% at 20 mA/cm², and a power efficiency (PE) of 7.56 cd/A. [1] An iridium complex containing a piq-derivative, Ir(piq-F)₂(acac), has been reported later and showed higher efficiency and brightness than those of Ir(piq)₂(acac). However, the emission of Ir(3Fpiq)₂(acac) exhibits a hypsochromic shift at 600 nm, compared to that of Ir(piq)₂(acac).

In this paper, we report a series of efficient red electrophosphorescent devices based on iridium complexes containing fluorinated 1-phenylisoquinoline (piq) derivatives are reported. To increase the efficiency and to tune the wavelength toward pure red, fluorinated piq derivatives are prepared and their OLEDs are fabricated. 3- and/or 4-position of the phenyl ring in piq were substituted with F to change the electronic property of the ligand in Ir complexes for phosphorescent efficiency or optimization to pure red emission. It is found that ligand substitution at 3- and 4-phenyl position leads to shift of electroluminescence (EL) wavelength. Further support on such emission peak shift is provided by theoretical calculation.

2. Experimental and Device Properties

The piq and its derivatives substituted with -F group were prepared by Suzuki coupling, as illustrated in (a) of Fig. 1. Iridium complexes were synthesized according to the method reported by Nonoyama with slight modification, as shown schematically in (b) of Fig.1.[2]

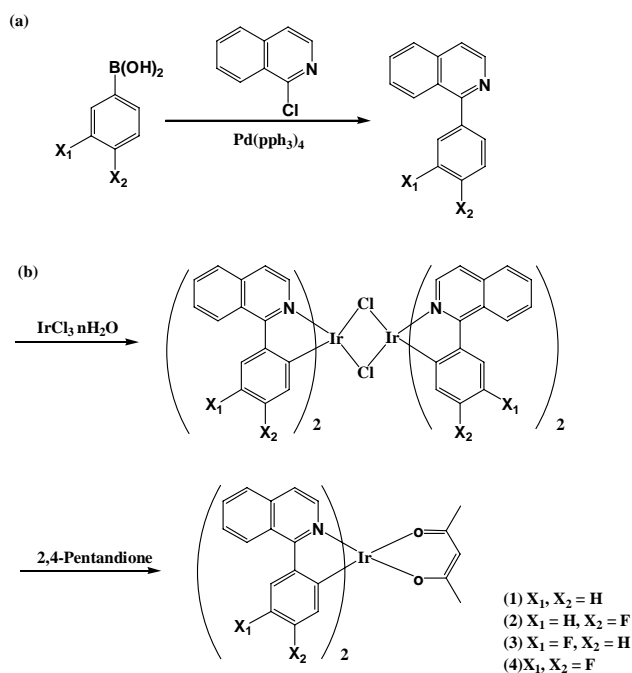


Fig. 1 (a) Synthesis of the piq ligand and its substituted derivatives [C^{^N}] (b) Synthesis of those Ir(III) complexes [Ir(C^{^N})₂(acac)]

The theoretical calculations of piq, fluorinated dpq ligands and their Ir(III) complexes were performed by *Ab initio* method. Density functional theory (DFT) utilizing B3LYP functional with the LANL2DZ and 6-

31G(d) basis sets for iridium and the other atoms, respectively, was used for energy calculation and geometry optimization for the ground electronic state. To obtain the vertical excitation energies of the low-lying singlet and triplet excited states of the complexes, time-dependent DFT (TD-DFT) calculations using the B3LYP functional was performed at the respective ground-state geometry, where the basis set of ligands was changed to 6-31+G(d). [3]

The OLEDs were fabricated by high vacuum (5×10^{-7} torr) thermal deposition of organic materials onto the surface of an indium tin oxide coated glass substrate. The ITO glass was chemically cleaned using acetone, methanol, distilled water and isopropyl alcohol. The organic materials were deposited in following sequence: 4,4',4''-tris[2-naphthyl phenylamino] triphenylamine (2-TNATA) (60 nm)/ 4,4'-bis[N-(naphthyl)-N-phenyl-amino]biphenyl (NPB) (20 nm)/10 % Ir complex in 4,4,N,N'-dicarbazolebiphenyl (CBP) (30 nm)/bathocuproine (BCP) (10 nm)/tris-(8-hydroxyquinoline) aluminum (Alq_3) (20 nm)/lithium quinolate (Liq) (2 nm)/Al (100). After the fabrication, the current density-voltage (J-V) characteristics of the OLEDs were measured with a source measure unit (Keithley 236) and the luminance and CIE chromaticity coordinates of the fabricated devices were measured by using a chromameter (MINOLTA CS-100A). All measurements were performed in ambient conditions under DC voltage bias.

3. Results and Discussions

An electron withdrawing group F is lower the energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) of the piq backbone. Thus, their substitution effects were investigated. Fig.2 shows the EL characteristics of devices with Ir complexes at the applied voltage of 12 V.

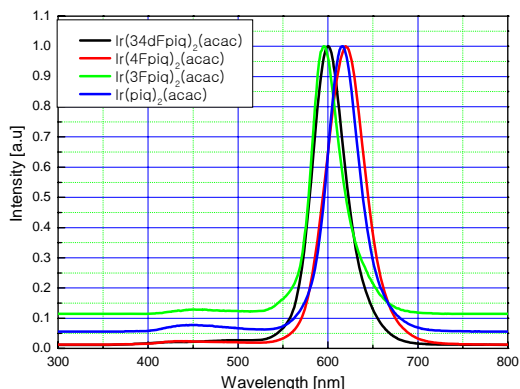


Fig. 2 EL spectra of the devices fabricated in this study at an applied voltage of 12 V.

$\text{Ir}(\text{piq})_2(\text{acac})$, $\text{Ir}(3\text{Fpiq})_2(\text{acac})$, $\text{Ir}(4\text{Fpiq})_2(\text{acac})$ and $\text{Ir}(34\text{dFpiq})_2(\text{acac})$ exhibit prominent EL emission at 616 nm, 595 nm, 619 nm and 600 nm, respectively. The variations of HOMO and LUMO levels change the energy gap between HOMO and LUMO, leading to such shift in emission wavelength. According to the substituted position of -F group in the ligand, the energy gap of the iridium complexes varied. Thus, the emission wavelengths of Ir(III) complexes could be tuned. Fig. 3 shows the luminous efficiencies of the devices as a function of the applied current densities.

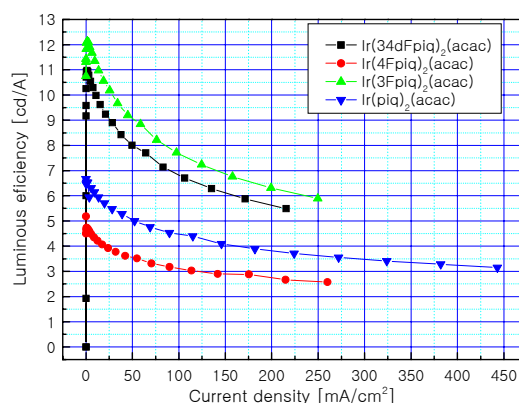


Fig. 3 The luminous efficiencies of the devices with the applied current densities.

The maximum efficiencies of the devices with $\text{Ir}(34\text{dFpiq})_2(\text{acac})$ dopants are similar to those of the devices with $\text{Ir}(3\text{Fpiq})_2(\text{acac})$, 10.97 cd/A at the current density of 1.06 mA/cm^2 and 12.13 cd/A at the current density of 1.45 mA/cm^2 , respectively. In addition, the CIE coordinate of $\text{Ir}(34\text{dFpiq})_2(\text{acac})$ (0.647, 0.351) is more reddish than that of $\text{Ir}(3\text{Fpiq})_2(\text{acac})$ (0.635, 0.363). The experimental results show that these complexes can be applied as red light emitting dopants in phosphorescent OLEDs.

Acknowledgements

This work was supported by City of Seoul Research Fund (2006) and Hongik University (2006).

References

- [1] Y.J.Su, H. L. Huang, C. L. Li, C. H Chien, Y. T. Tao, P. T. Chou, S. Datta and R. S. Liu Adv. Mater. **15**, 884 (2003)
- [2] H. H. Rho, G. Y. Park, Y. Ha and Y. S. Kim, Jpn. J. Appl. Phys., **45**, 568 (2006).
- [3] M. J. Frisch et. al.: Gaussian 98, Revision A.9, Gaussian, Inc., Pittsburgh, PA, 1988.