

## Study of bis{2-(naphtha [3,4]imidazol-2-yl) quinolinato} Magnesium

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**Abstract:** The study of bis{2-(naphtha[3,4]imidazol-2-yl) quinolinato} Magnesium (MgNIQ) is presented in this report. It was observed the decomposition temperature is high to 577°C but no melting transition ( $T_m$ ) of MgNIQ up to 450°C. By using of MgNIQ as emitted layer exhibits a broad maximum spectrum peak at 615 nm. The color of the emitted light is in the orange-red region in the CIE coordinate of  $x = 0.36$   $y = 0.53$ .

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**Keywords** Electroluminescence; red light; device; bis{2-(naphtha [3,4]imidazol-2-yl) quinolinato}

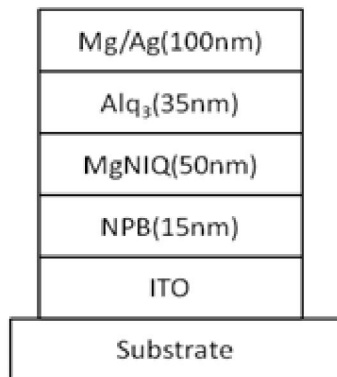
### 1. Introduction

Luminescent organic/organometallic compounds have attracted much attention recently because of their potential applications in electroluminescent (EL) displays [1-5]. Organic and polymer devices provide advantages over their inorganic counterparts, such as high luminous efficiency and fine-pixel formation. Luminescent chelate complexes have been shown to be particularly useful in electroluminescent (EL) displays because of their relatively high stability and volatility. The most well-known example of such chelate compounds is Alq<sub>3</sub>, not only a good emitter but also a highly efficient electron-transporting material, where q is the 8-hydroxyquinolinato ligand [6, 7]. Via the modification of the ligand of metal chelate compound, the emission color of a metal chelate compound may be tuned. Other properties, such as thermal stability and carrier mobility, may also be improved upon. In the present work, we report the synthesis and electroluminescent (EL) property of bis{2-(naphtha[3,4]imidazol-2-yl) quinolinato} Magnesium (MgNIQ). The attachment of the naphtha[3,4]imidazol group at 2-position would allow the ligand to form stable complexes with metal ions similarly to 8-hydroxyquinoline. Therefore, the thermal stability, an important character for the practical application in the electronic fields, of this metal complex is investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The organic emitting device using MgNIQ as emitting layer has been fabricated to study the electroluminescent property of this metal complex.

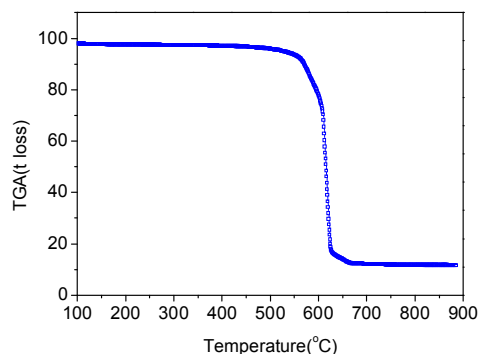
### 2. Experimental

The synthesis of the title compound was accomplished by following processes, as shown in Scheme 1. The dibutylmagnesium solution (0.5M in

heptane, 0.6927mL, 10mmol) was slowly added to 100 ml of THF solution containing 2-(naphtha[3,4]imidazol-2-yl) quinoline [8] (2.95g, 10mmol) at 0°C under N<sub>2</sub>. After the resulting mixture was stirred at room temperature for 6 hours, 5 ml isopropyl alcohol was added to quench the reaction. The solvents were removed under vacuum condition at  $5 \times 10^{-3}$  Torr, and the residual solid was sublimed to purify the final product. Orange powder of MgNIQ was obtained in 85% yield. The formula of this compound has been determined by <sup>1</sup>H NMR and elemental analysis. The organic light emitting device, Fig. 1, using MgNIQ as the emitting layer were fabricated on the transparent conductive indium-tin oxide (ITO) glass substrate. The organic layers and the cathode were sequentially deposited by conventional vacuum vapor deposition in the same chamber without breaking the vacuum under  $3 \times 10^{-7}$  Torr. In the present work, the N,N'-bis-(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine (NPB) was used as the hole-transport material (HTM), and tris (8-quinolinolato) aluminum (Alq<sub>3</sub>) was employed as the electron-transporting material (ETM). The EL spectrum and the Commission International de l'Eclairage (CIE) co-ordinates were measured by Pro-650 Spectroscanner (step size is 1.0 nm and bandpass is 4nm), the current-voltage (I-V) characteristic was measured by Keithley 2400 Source meter.

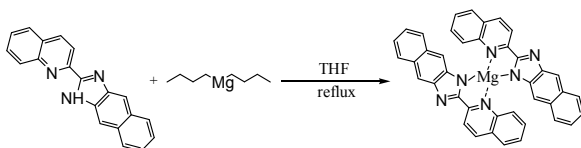


**Fig. 1.** Device structure of organic light emitting device (OLED) fabricated in this work



**Fig. 2.** TGA curve of MgNIQ.

### Scheme 1.



Thermogravimetric analysis (TGA) was performed on a Perkin-Elmer thermogravimeter (Pyris 1) under a dry nitrogen gas flow at the heating rate of 20°C/min. Glass transition temperature ( $T_g$ ) and melting point ( $T_m$ ) of materials were determined by differential scanning calorimetry of the Perkin-Elmer differential scanning calorimeter (DSC-7).

### 3. Results and discussion

Fig. 2 shows the TGA of MgNIQ that possesses a maximum rate of weight loss occurring at 577°C and no weight loss was observed at the temperature lower than 465°C. Above 600°C, there is about 13 wt % of residue composed of Magnesium ash. This Magnesium complex is reasonably stable upon exposure to air and exhibited a very high thermal stability in nitrogen, which is attributed to the fact that the Mg-N (imidazole) bond is highly polarized [9, 10]. The melting temperature ( $T_m$ ) of MgNIQ was not observed up to 450°C with DSC curve. The DSC and TGA results indicate that the MgNIQ possesses a very high thermal stability, which may serve as an advantage for the fabrication of organic light emitting device because the use of the materials with high thermal stability as the active emissive layer or carrier transporting layer may provide the device with greater longevity [11, 12].

The Photoluminescent (PL) spectra of the MgNIQ solutions and neat film, excited with 350 nm laser line, were illustrated in Figure 3. At low concentration,  $1 \times 10^{-5}$  M in DMF, only one emission band is observed with maximum at 489nm, corresponding to the relaxation of MgNIQ from the excited state of a single molecule into ground state. Besides the 489 nm band, a new emission band appeared while the concentration of MgNIQ increased from  $1 \times 10^{-5}$  to  $1 \times 10^{-3}$  M. This new emission band having a maximum at 565nm is observed in the spectrum of the MgNIQ neat film. We have assigned this new emission band to the excimer and higher aggregates emission [13, 14] resulting from the relaxation of collision complex into the lower energy state. The EL spectrum of organic light emitting device at the bias voltage of 13 V, Fig. 4, shows the broad emission band in the 500-700nm region with the maximum at 615nm. The emission is almost fixed in the orange-red region in the CIE coordinate of  $x = 0.36$   $y = 0.53$ , Fig. 5. For the small molecular organic materials, to develop the new type of material with red emission is very important because this kind of material is very seldom prepared so far, and it is very important for the fabrication of full color display panels. The change of the spectral wavelength may be achieved also by general conception of search and design of modified materials for wide band emission consists in substitution of the backside groups by electron acceptors like halogens etc. and different kind of donors [15, 16]. At the same time important role here may play electron-vibration interactions determining the spectral broadening of the emission lines. So the future strategy of the materials design may be in this way also.

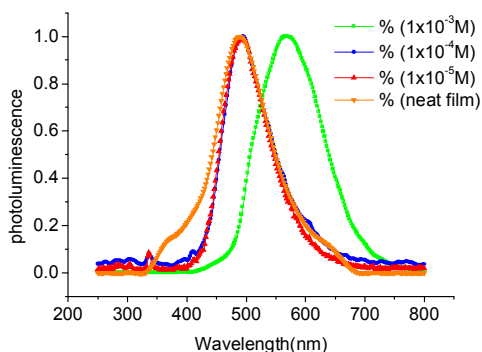


Fig. 3. Photoluminescent spectra of the MgNIQ in solutions and neat film

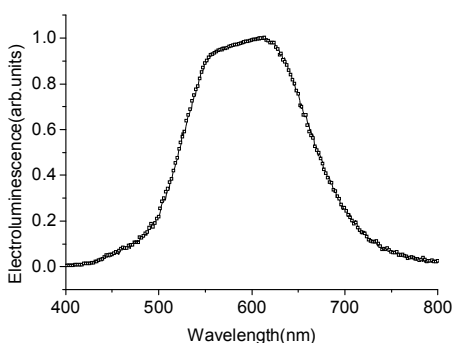


Fig. 4. EL spectrum of OLED fabricated in this work.

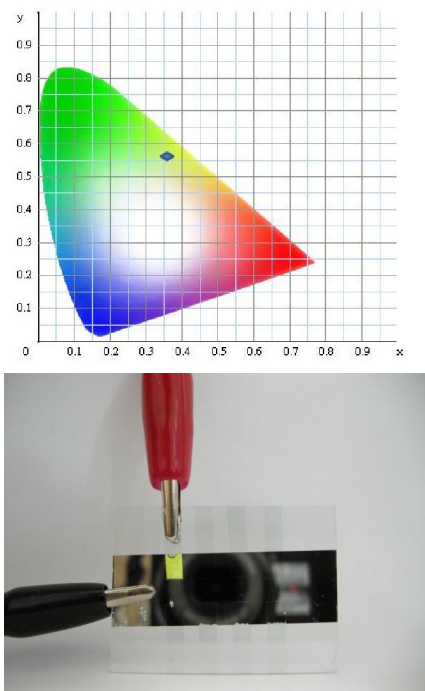


Fig. 5. CIE color coordinates (CIE<sub>x,y</sub> = 0.36,0.53) for the light emission produced by the OLED devices.

Figure 6 shows the energy level diagram of the HOMO and LUMO of the different organic materials and the work function of cathode and anode. The LUMO energy of MgNIQ is 2.6eV determined from the HOMO energy (5.8eV) obtained from the cyclic voltammetry (CV) method and the optical band gap estimated from the absorption onset. Comparing the energy level of MgNIQ with NPB, it is clear that the MgNIQ has the much higher hole injection barrier than that of NPB; in fact, it is impossible for the hole injection from ITO into MgNIQ without the assistance of NPB or some other kind of HTLs. This diagram also pointed out that the Alq<sub>3</sub> has the lower electron injection barrier than that of MgNIQ, so the electron injection from the MgAg into MgNIQ will be enhanced and confines the recombination zone at the interface between NPB and MgNIQ. Fig. 7 shows the current-voltage and luminance-voltage characteristics of this device having a low turn on voltage of about 6.0V for current and luminance. This device shows a brightness of 2414 cdm<sup>-2</sup> at the driving voltage of 13V with current density of 334 mA/cm<sup>2</sup>, decaying to 25 cdm<sup>-2</sup> in 120 hours.

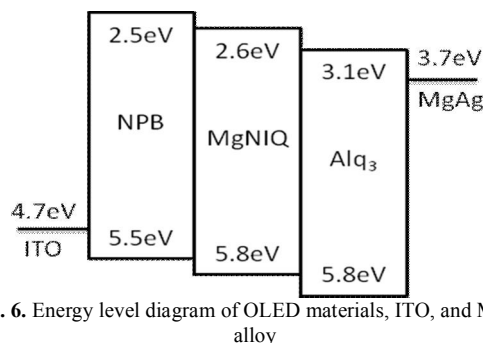


Fig. 6. Energy level diagram of OLED materials, ITO, and Mg-Ag alloy

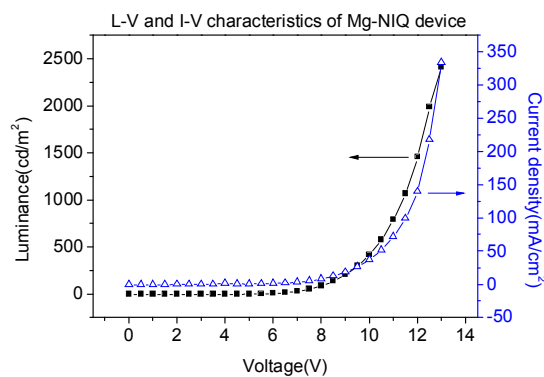


Fig.7. Current-voltage and luminance- voltage characteristics of OLED fabricated in this work.

#### 4. Conclusion

A novel metal complex, bis{2-(naphtha[3,4]imidazol-2-yl) quinolinato} magnesium (MgNIQ), was successfully prepared by the reaction of 2-(naphtha[3,4]imidazol-2-yl) quinoline and dibutyl-

magnesium. The investigation demonstrated that this compound possess charge transfer and film-forming properties and has high thermal stability.

The excimer emission resulting from the collision complex was observed. The devices composed of MgNIQ as the emitting layer can tune the emitting color via the controlling of carrier recombination region. Because of its high thermal stability and excellent electrical characteristics, MgNIQ and its related compound suggest a possible application for the use of the organic light emitting devices.

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