



Emitting materials based on phenylanthracene-substituted naphthalene derivatives for organic light-emitting diodes

Hyun Woo Lee^a, Hye Jeong Kim^a, Young Seok Kim^a, Jwajin Kim^a, Song Eun Lee^b,
Ho Won Lee^b, Young Kwan Kim^{b,*}, Seung Soo Yoon^{a,*,**}

^a Department of Chemistry, Sungkyunkwan University, Suwon 440-746, Republic of Korea

^b Department of Information Display, Hongik University, Seoul 121-791, Republic of Korea

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ABSTRACT

This study reports the emitting materials based on phenylanthracene-substituted naphthalene derivatives to achieve efficient electroluminescent properties for OLED applications. An OLED device using 4,4'-bis(10-phenylanthracen-9-yl)-1,1'-binaphthalene exhibited the blue emission with the CIE coordinates of (0.19, 0.16) and efficient electroluminescent properties with the luminance, power and external quantum efficiency of 1.70 cd/A, 0.79 lm/W and 1.26% at 20 mA/cm², respectively. Also, the other device using 1,4-bis(10-phenylanthracene-9-yl)naphthalene exhibited white emission with the CIE coordinates of (0.34, 0.43) at 7V, respectively. This device exhibits the luminance, power and external quantum efficiency of 2.22 cd/A, 1.13 lm/W and 0.86% at 20 mA/cm², respectively.

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1. Introduction

Over the past years, many organic electroluminescent materials have been developed to meet the conditions for full color displays and solid-state lighting [1–3]. Anthracene derivatives have been used for various organic electroluminescent emitters because of wide-energy bandgap, high quantum yield and good thermal stability for OLED applications [4–6]. However, an anthracene with the planar structure has strong close-packing and thus it is well known to decrease electroluminescent efficiencies and color purity.

Recently, various anthracene derivatives including bulky substituents at the anthracene 9- and 10-position have been investigated. The bulky substituents provide steric hinderance, which prevents intermolecular interactions and thus reduces the self-quenching effect, thereby improving the EL performance [7,8].

This paper reports the design and synthesis of emitting materials (**1** and **2**) based on phenylanthracene-substituted naphthalene derivatives to develop efficient OLEDs. In compounds **1** and **2**, two phenylanthracenes are connected through naphthalene and 1,1'-dinaphthalene, to study the effect of structural variations of the emitting materials on the EL performance of OLED devices using

them. Particularly, compound **2** has the 1,1'-binaphthalene linkage with the almost 90° twisted structure. This non-coplanar structure of compound **2** would effectively inhibit molecular aggregation and thus improve the EL efficiencies of OLEDs using compound **2** [9].

2. Experimental details

2.1. Synthesis and characterization

General procedure for the Suzuki cross coupling reaction: 9-phenylanthracen-10-yl-boronic acid (2.4 mol) and the corresponding aryl bromides such as 1,4-dibromonaphthalene and 4,4'-dibromo-1,1'-binaphthalene (1.0 mol), Pd(PPh₃)₄ (0.04 mol), aqueous 2.0 M Na₂CO₃ (10.0 mol), ethanol, and toluene were mixed in a flask. The mixture was refluxed for 4 h. After the reaction was completed, water was added to quench the reaction. After cooling, the crude solid was collected by filtration, washed with water and ethanol. The product was purified by recrystallization from CH₂Cl₂/EtOH.

¹H NMR and ¹³C NMR were recorded on a Varian Unity Inova 300Nb or Bruker Avance III 500 MHz NMR spectrometer. FT-IR spectra were recorded using a Bruker VERTEX70 FT-IR spectrometer. Low-resolution mass spectra were measured using a Jeol JMS-600W spectrometer in the APCI mode. Elemental analyses (EA) were determined by a Flash 2000 autoanalyzer.

* Corresponding author. Tel.: +82 2 320 1646; fax: +82 2 3141 8928.

** Corresponding author. Tel.: +82 31 290 7071; fax: +82 31 290 7075.

E-mail addresses: kimykw@wow.hongik.ac.kr (Y.K. Kim),
ssyoon@skku.edu (S.S. Yoon).

1,4-bis(10-phenylanthracene-9-yl)naphthalene (1). Yield: 96%. ^1H NMR (CDCl_3 , 500 MHz, δ): 7.83–7.81 (m, 5H), 7.74–7.72 (m, 4H), 7.67 (t, $J=7.0$ Hz, 3H), 7.63 (dd, $J=6.5$ Hz, 2H), 7.60 (t, $J=7.5$ Hz, 3H), 7.41–7.40 (m, 6H), 7.36 (d, $J=6.5$ Hz, 2H), 7.24–7.22 (m, 3H), 7.19–7.15 (m, 4H) FT-IR (ATR): ν 2972, 2867, 1739, 1493, 1368, 766, 735, 701 cm^{-1} . MS (APCI $^+$) (m/z): 632 [M^+]. Calcd for $\text{C}_{50}\text{H}_{32}$: C, 94.90; H, 5.10. Found: C, 93.36; H, 5.76.

4,4'-bis(10-phenylanthracen-9-yl)-1,1'-binaphthalene (2). Yield: 85%. ^1H NMR (CDCl_3 , 500 MHz, δ): 7.94 (d, $J=7.0$ Hz, 2H), 7.86 (d, $J=8.5$ Hz, 2H), 7.82–7.78 (m, 6H), 7.73–7.71 (m, 2H), 7.67 (t, $J=7.0$ Hz, 6H), 7.64–7.38 (m, 6H), 7.46–7.43 (m, 2H), 7.41–7.38 (m, 5H), 7.36 (d, $J=7.0$ Hz, 3H), 7.33–7.27 (m, 4H); ^{13}C NMR (CDCl_3 , 125 MHz, δ): 140.0, 139.1, 137.6, 136.8, 135.1, 133.8, 133.2, 131.4, 130.8, 128.8, 128.5, 127.9, 127.5, 127.2, 127.2, 127.1, 126.3, 126.2, 125.4, 125.3, 125.2 FT-IR (ATR): ν 2971, 2864, 1740, 1440, 1367, 855, 765, 700 cm^{-1} . MS (APCI $^+$) (m/z): 758 [M^+]. Calcd for $\text{C}_{60}\text{H}_{38}$: C, 94.95; H, 5.05. Found: C, 93.60; H, 5.06.

2.2. Physical measurements

The UV–vis absorption and photoluminescence spectra were measured in dichloromethane (10^{-5} M) using Shimadzu UV-1650PC and AMINCO–Bowman series 2 luminescence spectrometers. The fluorescence quantum yields of the emitting materials in thin solid film were determined using BDAVB film as a standard ($\Phi_{\text{f}}=0.30$ measured by the calibrated integration sphere system) at 293 K [9]. The fluorescence quantum yields of the emitting materials were determined in dichloromethane at 293 K against DPA (9,10-diphenylanthracene) as a reference ($\Phi_{\text{DPA}}=0.90$) [10]. The HOMO (highest occupied molecular orbital) energy levels were measured with a low energy photo-electron spectrometer (Riken-Keiki, AC-2). The energy band gaps were determined from the intersection of the absorption and photoluminescence spectra. The LUMO (lowest unoccupied molecular orbital) energy levels were estimated by subtracting the corresponding optical band gap energies from the HOMO energy values. Thermogravimetric analysis (TGA) was carried out using a SEIKO EXSTAR 6000 TG/ DTA 7300 unit under a nitrogen atmosphere at a heating rate of 10 $^{\circ}\text{C}/\text{min}$.

2.3. OLED fabrication and measurement

For fabricating OLEDs, the indium–tin–oxide (ITO) thin films coated on glass substrates were used, which was 30 Ω/square of the sheet resistivity and 1000 \AA of thickness. The ITO coated glass was cleaned in an ultrasonic bath by the following sequences: in acetone, methyl alcohol, distilled water and kept in isopropyl alcohol for 48 h and dried by N_2 gas gun. The substrates were treated by O_2 plasma treatment with the conditions of 2×10^{-2} Torr at 125 W for 2 min. All organic materials and metal were deposited under high vacuum (5×10^{-7} Torr). The OLEDs were fabricated in the following sequence: ITO/4,4'-Bis(N-(1-naphthyl)-N-phenylamino)biphenyl (NPB) (50 nm)/emitting materials (**1** and **2**) (40 nm)/Tris(8-hydroxyquinolino)aluminum (Alq_3) (15 nm)/Lithium quinolate (Liq) (2 nm)/Al (100 nm). All

of the properties of the OLEDs such as current density (J), luminance (L), luminous efficiency (LE), and the CIE chromaticity coordinates of OLEDs were measured with Keithly 2400, Chroma meter CS-1000A. Electroluminescence was measured using Roper Scientific Pro 300i.

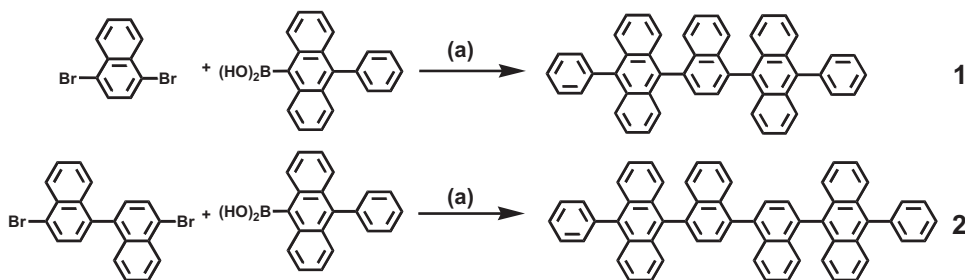
3. Results and discussion

Scheme 1 shows the structures and synthetic route of compounds **1** and **2**. Compounds **1** and **2** were synthesized by using the common Suzuki cross coupling reactions between 9-phenylanthracen-10-yl-boronic acid and the corresponding aryl bromides in moderate yields. All the compounds were characterized by ^1H NMR, IR, mass spectroscopy and elemental analysis. High-performance liquid chromatography was carried out to check the purity of the materials. These analyses revealed that the purity of these materials was at least above 99.5%.

The thermal properties of compounds **1** and **2** using DSC and TGA measurements are shown in **Table 1**. It exhibits no observable glass transition temperatures (T_g) and melting temperatures (T_m) at temperature below 350 $^{\circ}\text{C}$. Decomposition temperatures (T_d) were observed high values of 422 and 452 $^{\circ}\text{C}$ (DPA $T_d=241$ $^{\circ}\text{C}$), respectively. It suggests that compounds **1** and **2** have high thermal stabilities.

Fig. 1(a) shows the UV–vis absorption spectra of compounds **1** and **2** in dichloromethane. PL emission spectra of compounds **1** and **2** are shown in **Fig. 1(b)** in dichloromethane and **Fig. 1(c)** in quartz plates. In the UV–vis absorption spectra, the maximum absorption wavelengths of compounds **1** and **2** appeared at 398 and 396 nm, respectively. Absorption spectra have similar absorption peaks and shapes of 350–400 nm due to the characteristic vibration patterns of an isolated anthracene groups ($\lambda_{\text{max}}=357, 375, 397$ nm). In the PL spectra in dichloromethane, the maximum emission wavelengths (λ_{max}) of compounds **1** and **2** appeared at $\lambda_{\text{max}}=410$ and 411 nm, respectively, in the blue region of the visible spectrum. PL spectra of compounds **1** and **2** in film showed red-shifted emission around 21 and 31 nm due to the solid-state packing effects [11]. The emission quantum yields of compounds **1** and **2** were high ($\Phi=0.79$ and 0.75), suggesting that compounds **1** and **2** would have high efficient electroluminescent properties in OLED devices. The highest occupied molecular orbital (HOMO) levels were measured using a photoelectron spectrometer (Riken-Keiki AC-2) and the lowest unoccupied molecular orbital (LUMO) levels calculated by subtracting the corresponding optical band gap energies from the HOMO values. The HOMO energy levels of compounds **1** and **2** were -5.88 and -5.87 eV, respectively (**Table 1**). The LUMO energy levels for these materials which are calculated by HOMO–LUMO energy gaps were -2.72 and -2.71 eV, respectively. These results are summarized in **Table 1**.

Density functional theory (DFT) of compounds **1** and **2** were carried out using the Becke's three parameterized Lee–Yang–Parr (B3LYP) functional with 6-31G* basis sets using a suite of Gaussian programs to understand the observed optical properties of the organic light-



Scheme 1. Structures and synthetic routes of compounds **1** and **2**. (a) 9-phenylanthracen-10-yl boronic acid, (a) $\text{Pd}(\text{PPh}_3)_4$, 2M Na_2CO_3 , toluene, ethanol.

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