



# Synthesis and electroluminescent properties of *tert*-butylated arylamine substituted 9,10-diphenylanthracene derivatives for organic light-emitting diodes



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## ABSTRACT

This paper reports synthesis and electroluminescent properties of the *tert*-butylated arylamine-substituted 9,10-diphenylanthracene derivatives for organic light-emitting diodes. The devices using these materials were fabricated in the following sequence: indium-tin-oxide/*N,N'*-di(1-naphthyl)-*N,N'*-diphenyl-(1,1'-biphenyl)-4,4'-diamine/emitting material/bathophenanthroline/lithium quinolate/aluminum. All devices showed the efficient electroluminescence depending on the photoluminescent properties of emitters. In particular, a device using 2-*tert*-butyl-9-(9,10-diphenylanthracen-2-yl)-9*H*-carbazole exhibited blue emission with the maximum luminance, luminous efficiency, power efficiency and external quantum efficiency of 2552 cd/m<sup>2</sup>, 2.14 cd/A, 1.17 lm/W and 2.04% at 20 mA/cm<sup>2</sup>, respectively, and Commission Internationale d'Éclairage (CIE) coordinates of (0.15, 0.12) at 6.0 V. These results suggest that the degree of self-aggregation of the emitters and charge-balances in the emitting layers of devices would be important roles in electroluminescent properties of devices.

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## 1. Introduction

In the past years, organic light-emitting diodes (OLEDs) have attracted great attentions in industrial and academic fields due to their potential of applications such as full-color, large-area, flat-panel, flexible, and transparent displays as well as solid state lighting. The OLED technology has been developed in the aspect of materials research and device fabrication performance since the influential studies on the OLEDs by Tang and VanSlyke in 1987 [1]. However, blue fluorescent materials which have intrinsic characteristic of wide energy band gap still needed to be further studied to enhance their stability, color purity, lifetime, and efficiencies simultaneously for full-color OLED displays [2–4].

Meanwhile, anthracene derivatives have been extensively studied and developed as blue light-emitting materials in OLEDs because of their outstanding photoluminescence (PL) and electroluminescence (EL) properties [5]. Especially, 9,10-diphenylanthracene (DPA) is an attractive material in terms of its high quantum

yield ( $\Phi = 0.90$ ) in dilute solution [6]. However, the EL properties of solid state OLEDs using this material are decreased due to the self-aggregation among the molecules. Besides, it tends to form crystallized state, which makes film state to be heterogeneous and increases the resistance of the emitters in thin films.

In previous works, there have been many reports on 9,10-diphenylanthracene-derived blue emitters with the substituents at *para*-position of diphenyl moieties such as fluorene, naphthalene [7,8], carbazole [9,10], or triphenylvinyl [11,12]. Also, the blue emitters with the substitutions at C-2 position of anthracene core of 9,10-diphenylanthracene such as arylamine, triphenylsilane, diphenylphosphine oxide, or dimesitylborane [13,14] have been studied.

As the extension of these efforts, we designed and synthesized the emitting materials (**1–4**) based on 9,10-diphenylanthracene backbone end-capped with *tert*-butylated diphenylamine and carbazole groups at C-2 position of anthracene core. The non-planar structures of these materials, which were originated from the twisted linkage between anthracene backbone and arylamino groups, and *tert*-butyl group at the arylamino groups would reduce the intermolecular interaction and prevent self-aggregation and concentration quenching by the excimer [15,16]. This would lead to

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the improved EL efficiencies of devices using them as the emitting materials. Moreover, diphenylamine and carbazole derivatives were brought in to improve device performances using them due to their improved hole transporting properties [17,18].

## 2. Experimental details

### 2.1. Synthesis and characterization

2-Bromo-9,10-diphenylanthracene and 2,6-dibromo-9,10-diphenylanthracene was synthesized according to literature [14].  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR were recorded on Bruker Avance III 500 MHz NMR spectrometer. FT-IR spectra were recorded using a Bruker VERTEX70 FT-IR spectrometer. Low and high-resolution mass spectra were measured using Jeol JMS-AX505WA spectrometer in ACPI mode. Elemental analysis (EA) was measured using an EA 1108 spectrometer.

#### 2.1.1. 2-tert-Butyl-9-(9,10-diphenylanthracen-2-yl)-9H-carbazole (1)

2-Bromo-9,10-diphenylanthracene (0.98 mmol), 2-tert-butyl-9H-carbazole (1.07 mmol),  $\text{Pd}_2(\text{dba})_3$  (0.05 mmol), tri-tert-butylphosphine (0.05 mmol), sodium tert-butoxide (1.95 mmol), and anhydrous toluene 20 ml were mixed in a flask. The mixture was refluxed for 4 h at 120 °C. After the reaction finished, the reaction mixture was extracted with toluene and washed with water. The organic layer was dried with anhydrous  $\text{MgSO}_4$  and filtered with silica gel. The solution was then evaporated. The crude product was purified by recrystallization from  $\text{CH}_2\text{Cl}_2/\text{EtOH}$ . (Yield: 64%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 8.06 (d,  $J=8.0$  Hz, 1H), 8.01 (d,  $J=8.0$  Hz, 1H), 7.93 (d,  $J=9.5$  Hz, 1H), 7.90 (s, 1H), 7.77–7.70 (m, 2H), 7.66 (t,  $J=8.0$  Hz, 1H), 7.61–7.55 (m, 4H), 7.53–7.52 (m, 4H), 7.47 (s, 1H), 7.45–7.43 (m, 2H), 7.39–7.37 (m, 2H), 7.34–7.31 (m, 2H), 7.22 (d,  $J=7.0$  Hz, 1H), 1.35 (s, 9H);  $^{13}\text{C}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 149.7, 140.7, 140.4, 138.8, 138.6, 137.5, 137.1, 134.3, 131.3, 131.1, 130.5, 130.3, 130.2, 129.1, 128.6, 127.7, 127.1, 126.9, 125.6, 125.4, 125.3, 124.4, 123.4, 123.4, 121.1, 121.0, 120.0, 120.0, 119.7, 118.7, 118.1, 117.8, 109.8, 106.2, 35.2, 31.7; FT-IR [ATR]:  $\nu$  ( $\text{cm}^{-1}$ ) 3055, 2397, 2351, 2282, 1607, 1544, 1493, 1462, 1428, 1351, 1229, 861, 834, 747, 699; APCI-MS ( $m/z$ ): 551 [ $\text{M}^+$ ]; Anal. Calcd: C, 91.43; H, 6.03; N, 2.54. Found: C, 91.21; H, 5.98; N, 2.51.

#### 2.1.2. 2-tert-Butyl-9-(4-(9,10-diphenylanthracen-2-yl)phenyl)-9H-carbazole (2)

2-Bromo-9,10-diphenylanthracene (0.98 mmol), 2-tert-butyl-9-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-9H-carbazole (1.03 mmol) and,  $\text{Pd}(\text{PPh}_3)_4$  (0.04 mmol), aqueous 2.0 M  $\text{Na}_2\text{CO}_3$  (2.93 mmol), toluene 3 ml, and ethanol 1.5 ml were mixed in a flask. The mixture was refluxed for 2 h at 120 °C. After the reaction finished, the reaction mixture was extracted with ethyl acetate and washed with water. The organic layer was dried with anhydrous  $\text{MgSO}_4$  and filtered with silica gel. The solution was then evaporated. The crude product was purified by recrystallization from  $\text{CH}_2\text{Cl}_2/\text{EtOH}$ . (Yield: 80%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 8.09 (d,  $J=7.5$  Hz, 1H), 8.06–8.04 (m, 2H), 7.85 (d,  $J=9.0$  Hz, 1H), 7.79 (d,  $J=8.5$  Hz, 2H), 7.74–7.71 (m, 3H), 7.67–7.64 (m, 4H), 7.61–7.54 (m, 8H), 7.45 (s, 1H), 7.41 (d,  $J=8.0$  Hz, 1H), 7.38–7.34 (m, 4H), 1.38 (s, 9H);  $^{13}\text{C}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 149.8, 141.1, 140.9, 139.8, 138.9, 138.9, 137.6, 137.1, 137.0, 136.3, 131.4, 131.3, 130.4, 130.1, 130.0, 129.1, 128.6, 128.6, 128.5, 127.9, 127.7, 127.6, 127.3, 127.0, 127.0, 125.4, 125.3, 125.2, 124.8, 124.5, 123.4, 121.0, 120.0, 119.8, 119.8, 118.1, 109.7, 106.2, 35.3, 31.8; FT-IR [ATR]:  $\nu$  ( $\text{cm}^{-1}$ ) 3069, 2964, 1739, 1494, 1457, 1388, 1336, 1235, 1026, 960, 820, 750, 728, 701; APCI-MS ( $m/z$ ): 627 [ $\text{M}^+$ ]; Anal. Calcd: C, 91.93; H, 5.94; N, 2.23. Found: C, 91.74; H, 5.89; N, 2.21.

#### 2.1.3. 2-tert-Butyl-9-(2-(2-tert-butyl-9H-carbazol-9-yl)-9,10-diphenylanthracen-6-yl)-9H-carbazole (3)

(Yield: 43%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 8.08 (d,  $J=7.5$  Hz, 2H), 8.04 (d,  $J=8.5$  Hz, 2H), 7.96–7.95 (m, 2H), 7.94 (s, 1H), 7.64–7.61 (m, 6H), 7.58 (t,  $J=7.5$  Hz, 4H), 7.49–7.48 (m, 3H), 7.47–7.46 (m, 3H), 7.37–7.34 (m, 4H), 1.37 (s, 18H);  $^{13}\text{C}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 136.7, 136.2, 135.8, 134.4, 133.8, 132.8, 132.7, 132.4, 131.0, 128.7, 128.4, 127.2, 127.1, 126.3, 125.4, 124.4, 123.5, 122.9, 122.6, 121.0, 120.6, 119.9, 119.8, 109.8, 95.5, 31.9; FT-IR [ATR]:  $\nu$  ( $\text{cm}^{-1}$ ) 3019, 2966, 1621, 1598, 1427, 1353, 1227, 816, 789, 747, 700; APCI-MS ( $m/z$ ): 773 [ $\text{M}^+$ ]; Anal. Calcd: C, 90.12; H, 6.26; N, 3.62. Found: C, 90.07; H, 6.19; N, 3.59.

#### 2.1.4. N-(4-tert-Butylphenyl)-N,9,10-triphenylanthracen-2-amine (4)

(Yield: 71%).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 7.66–7.62 (m, 2H), 7.68 (t,  $J=8.0$  Hz, 2H), 7.64–7.61 (d, 2H), 7.48 (d,  $J=8.0$  Hz, 2H), 7.36 (t,  $J=7.0$  Hz, 2H), 7.23–7.18 (m, 4H), 7.15 (d,  $J=8.0$  Hz, 1H), 7.07 (m, 3H), 7.01–6.96 (m, 3H), 1.31 (s, 9H);  $^{13}\text{C}$  NMR (500 MHz,  $\text{CDCl}_3$ ) [ $\delta$  ppm]; 147.9, 147.5, 143.6, 142.9, 140.6, 140.1, 139.8, 138.9, 136.7, 136.6, 136.1, 134.6, 130.6, 130.2, 129.6, 129.0, 128.4, 128.1, 127.9, 127.8, 127.7, 127.3, 127.2, 127.1, 127.0, 126.5, 124.7, 124.0, 123.2; FT-IR [ATR]:  $\nu$  ( $\text{cm}^{-1}$ ) 3061, 1624, 1596, 1495, 1453, 1322, 1270, 1072, 1025, 857, 824, 758, 702; APCI-MS ( $m/z$ ): 553 [ $\text{M}^+$ ]; Anal. Calcd: C, 91.10; H, 6.37; N, 2.53. Found: C, 89.93; H, 6.19; N, 2.49.

### 2.2. Physical measurements

The UV–vis absorption and photoluminescence spectra of these synthesized materials were measured in dichloromethane ( $10^{-5}$  M) using Shimadzu UV-1650PC and Amincobrowman series 2 luminescence spectrometers. The fluorescent quantum yield were determined in dichloromethane solution at 293 K against 9,10-diphenylanthracene (DPA) as a reference ( $\Phi=0.90$ ) [19]. The HOMO (highest occupied molecular orbital) energy levels were measured with a low energy photo-electron spectrometry (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 energy band gap from the HOMO energy levels.

### 2.3. OLED fabrication and measurement

For fabricating OLEDs, the indium-tin-oxide (ITO) thin films coated on glass substrates were used, which was  $30 \Omega/\text{square}$  of the sheet resistivity. 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  $\text{N}_2$  gas gun. The substrates were treated by  $\text{O}_2$  plasma treatment with the conditions of  $2 \times 10^{-2}$  Torr at 125 W for 2 min. All organic materials and metal were deposited under high vacuum ( $5 \times 10^{-7}$  Torr). The OLEDs were fabricated in the following sequence: ITO (180 nm)/N,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) (50 nm)/blue light-emitting materials (1–4) (30 nm)/bathophenanthroline (Bphen) (30 nm)/lithium quinolate (Liq):Al (100 nm) (Devices A–D). 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. Electro luminance was measured using Roper Scientific Pro 300i.

## 3. Results and discussion

Compounds 1–4 were synthesized by Buchwald–Hartwig cross-coupling or Suzuki cross-coupling reactions as shown in

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