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High-color-purity and high-efficiency non-doped deep-blue electroluminescent devices based on novel anthracene derivatives[†]

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Two novel anthracene derivatives 2-*tert*-butyl-9,10-bis(2-biphenyl) anthracene (TBBPA) and 2-*tert*-butyl-9,10-bis[2-(1-naphthyl)phenyl]anthracene (TBNPA) were synthesized and characterized. The quantum chemical calculations show that TBBPA and TBNPA have highly non-coplanar structures. Both the two anthracene derivatives exhibit deep-blue emission with high fluorescence quantum yields. The electrochemical properties and energy levels of the two compounds were investigated by cyclic voltammetry. The non-doped devices based on the two anthracene derivatives exhibit low turn-on voltage and stable deep-blue emission with high efficiency (external quantum efficiency of about 3.0%). The Commission Internationale de l'Eclairage (CIE) coordinates (0.15, 0.07) of the devices are very close to the National Television System Committee (NTSC) blue standard. The comprehensive performances of the devices are comparable to the best of the non-doped deep-blue OLEDs with a CIE coordinate of y < 0.10.

Introduction

Since the pioneering work on organic light emitting devices (OLEDs) by the Kodak group,¹ OLEDs have been attracting considerable attention due to their potential applications in flat-panel displays and solid-state lighting sources.^{1–5} For the full-color OLEDs, highly efficient and stable three basic color (red, green, and blue) emissions are needed. Although OLEDs have achieved remarkable development to date, the performance of blue OLEDs is often inferior to those of red and green ones because of the intrinsic wide band gap of blue-emitting materials.⁶⁻⁸ The electroluminescence (EL) efficiency can be improved by using dopant emitters, but the addition of dopants implies additional complexity and cost for the mass production of OLEDs. In addition to efficiency and stability, color purity is another important criterion for OLEDs. The Commission Internationale de l'Eclairage (CIE) coordinates of blue emission specified by the National Television System Committee (NTSC) are (0.14, 0.08). In addition, the power consumption of a full-color OLED is highly dependent upon the color of blue emission, and the deeper the blue color (smaller CIE y-value) is, the lower the power consumption of the device is.9 Thus, developing highly efficient

and stable non-doped deep-blue OLEDs continues to receive considerable attention. $^{10\mathac{-}16}$

It is well known that 9,10-diphenylanthracene (DPA) is an attractive material for its high fluorescence quantum efficiency in dilute solution.¹⁷ Nevertheless DPA is incapable of forming stable amorphous thin film because of its tendency to crystallize in the solid state, and its fluorescence can be easily quenched in the solid state, which hamper its application in OLEDs. 7,8,18,19 Moreover, to obtain excellent color purity, blue emitting materials should have molecular structures that can prevent excimer or exciplex formation which brings about broad and red-shifted electroluminescent emission.²⁰ To mitigate these problems, several deep-blue anthracene derivatives have been synthesized by introducing bulky groups at the para-position or meta-position of phenyl substituents in DPA.7,8,12,14,20-23 In this study, we designed and synthesized two novel anthracene derivatives 2-tert-butyl-9,10-bis(2-biphenyl) anthracene (TBBPA) and 2-tertbutyl-9,10-bis[2-(1-naphthyl)phenyl]anthracene (TBNPA).²⁴ In TBBPA and TBNPA, the phenyl group and naphthyl group were introduced at the ortho-position of phenyl substituents in DPA. This can further enhance the non-planarity of molecular structures and reduce the conjugation length of material molecules due to the higher steric hindrance. The introduction of the tert-butyl group in the anthracene unit can improve the performances of devices by reducing the molecular aggregation.²⁵ The quantum chemical calculations were carried out to investigate their stereostructures and electronic structures. The photophysical properties and electrochemical properties of the compounds were studied in a contrastive manner. The non-doped devices, ITO/bis[N-(1-naphthyl)-N-phenylamino]biphenyl (NPB, 30 nm)/TBBPA

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or TBNPA (30 nm)/1,3,5-tris(*N*-phenylbenzimidazol)benzene (TPBI, 30 nm)/LiF (2 nm)/Al, show stable deep-blue emission with high EL efficiency. The 1931 CIE coordinates (0.15, 0.07) of the devices are very close to the NTSC blue standard.

Experimental

General

Commercially available reagents were used without purification unless otherwise stated. ¹H NMR spectra were recorded in CDCl₃ solution on a Bruker Avance 400 spectrometer with tetramethylsilane (TMS) as the internal standard. Elemental analysis was performed on a Vario III elemental analyzer. Mass spectrum was obtained on a Bruker Microflex spectrometer. The absorption and photoluminescence spectra were recorded on a Hitachi U-3010 UV-Vis spectrophotometer and a Hitachi F-4500 fluorescence spectrophotometer, respectively. Cyclic voltammetry was performed on a CHI620C electrochemical analyzer.

Synthesis

2-*tert*-Butyl-9,10-dibromoanthracene (compound **2**) and 1-(2bromophenyl)naphthalene (compound **5**) were synthesized according to the literature.^{26,27} TBBPA and TBNPA were synthesized by the Suzuki coupling reaction (Scheme 1).

2-tert-Butyl-9,10-dibromoanthracene (2). Br₂ (3.2 g, 20 mmol) in 50 mL CCl₄ was added dropwise in 2-*tert*-butylanthracene **1** (2.3 g, 10 mmol) in 50 mL CCl₄ during stirring, then reacted for 12 h at room temperature. The precipitate was collected by filtration, and recrystallized from ethanol to give the yellow needle-like crystals (yield: 2.4 g, 62%). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.57–8.45 (4H, m), 7.74–7.72 (1H, d, J = 8.0), 7.62–7.60 (2H, m), 1.49 (9H, s); TOF-MS: m/z = 391.9; anal. calcd. for C₁₈H₁₆Br₂: C, 55.13; H, 4.11; found: C, 54.95; H, 4.03.

1-(2-Bromophenyl)naphthalene (5). Naphthalene-1-boronic acid **3** (1.7 g, 10 mmol), 1-iodo-2-bromobenzene **4** (2.82 g, 10 mmol), and tetrakis(triphenylphosphine)palladium [Pd(PPh₃)₄] (150 mg) were mixed in toluene (100 mL), then Na₂CO₃ (2 M, 30 mL) and ethanol (30 mL) were added during stirring, the mixture reacted for 24 h at 80 °C under the nitrogen atmosphere. After cooling, the resulting solution was extracted with CH₂Cl₂ three times, then the combined organic solution was dried over anhydrous MgSO₄ and evaporated with a rotary evaporator. The crude product was purified by column chromatography (eluent = *n*-hexane) to give a white powder (yield: 2.4 g, 85%). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.91–7.89 (2H, d, J = 8.0), 7.74–7.72 (1H, d, J = 8.0), 7.55–7.24 (8H, m); TOF-MS: *m/z* = 282.0; anal. calcd. for C₁₆H₁₁Br: C, 67.87; H, 3.92; found: C, 67.78; H, 3.84.

Biphenyl-2-boronic acid (7) and 1-(1-naphthyl)phenyl-2boronic acid (8). *n*-Butyl lithium (2.5 M, 6 mmol) was added dropwise to the solution of 6 (1.2 g, 5 mmol) or 5 (1.4 g, 5 mmol) in anhydrous THF (30 mL) at -78 °C during half an hour, and the mixture was stirred for another 1 h at this temperature. Trimethylborate (1.25 g, 12 mmol) was added to



Scheme 1 Synthetic route of TBBPA and TBNPA.

the reaction mixture at -78 °C, and stirred for 12 h at room temperature. Then HCl (2 M, 10 mL) was added, and stirred for 1 h. The resulting solution was extracted with CH₂Cl₂ three times, then the combined organic solution was dried over anhydrous MgSO₄ and evaporated with a rotary evaporator. The crude product was purified by column chromatography (eluent = dichloromethane/*n*-hexane, 1 : 3 v/v) to give a white powder (yield: 0.67 g, 68% for compound 7; 0.63 g, 51% for compound **8**). Compound 7: ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.94–7.92 (1H, d, J = 8.0), 7.50–7.40 (7H, m), 7.32–7.30 (1H, d, J = 8.0), 4.32 (2H, s); TOF-MS: m/z = 198.2.

2-*tert*-Butyl-9,10-bis(2-biphenyl) anthracene (TBBPA). 2-*tert*-Butyl-9,10-dibromoanthracene 2 (0.39 g, 1.0 mmol), biphenyl-2-boronic acid 7 (0.49 g, 2.5 mmol), and tetrakis-(triphenylphosphine)palladium [Pd(PPh₃)₄] (30 mg) were mixed in toluene (20 mL), then Na₂CO₃ (2 M, 5 mL) and ethanol (5 mL) were added during stirring. The mixture was refluxed under the nitrogen atmosphere for 24 h. After cooling, the precipitate was collected by filtration and purified by column chromatography (eluent = dichloromethane/*n*-hexane, 1:10 v/v). The product was recrystallized in toluene (yield: 0.28 g, 52%). ¹H NMR (400 MHz, CDCl₃) δ (ppm): 7.66–7.52 (6H, m), 7.49–7.45 (3H, m), 7.37–7.30 (3H, m), 7.29 (1H, s), 7.23–7.17 (2H, m), 6.99 (2H, d, J = 6.4), 6.94 (2H, d, J = 7.2), 6.94–6.80 (6H, m), 1.19 (9H, s); TOF-MS: m/z = 538.3; anal. calcd. for C₄₂H₃₄: C, 93.64; H, 6.36; found: C, 93.46; H, 6.27.

2-tert-Butyl-9,10-bis[**2-(1-naphthyl)phenyl]anthracene (TBNPA).** The synthesis of TBNPA is similar to that of TBBPA by a reaction of **2** with **8**, yield: 0.26 g, 41%. ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.24 (2H, d, J = 8.0), 8.13–7.86 (6H, m), 7.82–7.59 (7H, m), 7.46–7.32 (2H, m), 7.07–7.02 (3H, m), 6.88–6.76 (2H, m), 6.67 (1H, d, J = 8.0), 6.62–6.53 (2H, m), 6.51–6.42 (4H, m), 1.18 (9H, s); TOF-MS: m/z = 638.3; anal. calcd. for C₅₀H₃₈: C, 94.00; H, 6.00; found: C, 93.83; H, 5.92.

Devices fabrication and measurements. Indium-tin-oxide (ITO) coated glass substrates were cleaned with isopropyl alcohol and deionized water, then dried in an oven at 120 °C, and finally treated with UV-ozone. The devices were prepared in a vacuum at a pressure of about 1×10^{-6} Torr. Organic layers were deposited onto the substrate at a rate of 0.1–0.2 nm s⁻¹. After the organic film deposition, LiF and aluminum were thermally evaporated onto the surface of organic layer. The thicknesses of the organic materials and the cathode layers were controlled using a quartz crystal thickness monitor. EL spectra and 1931 CIE color coordinates were measured with a spectrascan PR650 photometer and the current–voltage–luminance characteristics were measured with a computer-controlled Keithley 2400 SourceMeter under ambient atmosphere.

Results and discussion

Quantum chemical calculations

Quantum chemical calculations were carried out to characterize the stereostructures and electronic structures of each material by using the B3LYP/6-31G(d) method.²⁸ The stereostructures of TBBPA and TBNPA are shown in Fig. 1. In TBBPA, the two benzene rings at the 9- and 10-positions are highly twisted towards the anthracene backbone to angles of 77.9° and 76.8° , respectively, and the dihedral angle between benzene rings in biphenyl groups is 53.1° (Fig. 1a). For TBNPA, the dihedral angles between aromatic rings are slightly larger than those of TBBPA (Fig. 1b). The calculation results indicate that the TBBPA and TBNPA have highly non-coplanar structures, which can limit the intermolecular interactions against fluorescence quenching and facilitate the formation of stable amorphous thin films. As shown in Fig. 1, the calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) electron densities of the materials are almost concentrated on the anthracene moiety. Thus, it is expected that the absorption and emission properties of TBBPA and TBNPA are controlled mostly by $\pi - \pi^*$ transition of the anthracene moiety.

Photophysical properties

Fig. 2 shows the absorption and photoluminescence (PL) spectra of TBBPA and TBNPA in dilute CH₂Cl₂ solutions. The absorption spectra of the compounds show the characteristic vibrational patterns of the isolated anthracene moiety (λ_{max} are about 341, 361, 379 and 399 nm).^{18,19} The additional absorption bands between 250 nm and 340 nm can be assigned



Fig. 1 Calculated stereostructures and frontier orbitals of TBBPA (a) and TBNPA (b).

to the groups at the 9- and 10-positions of the central anthracene core. When TBBPA is excited at either 379 nm or 265 nm, the same PL spectrum (λ_{max} are 421 nm and 443 nm) was observed. In the case of TBNPA, the same PL spectrum (λ_{max} are 425 nm and 443 nm) can be obtained by excitation at either 379 nm or 265 nm. It can be found that the structures of absorption and PL spectra of the compounds are similar to those of DPA (Fig. 2). The PL quantum yields in dilute CH₂Cl₂ solutions were measured to be 0.73 for TBBPA and 0.69 for TBNPA, respectively, by using DPA as the



Fig. 2 Absorption and photoluminescence spectra of TBBPA (a) and TBNPA (b) in dilute CH₂Cl₂ solution and solid thin film.

reference standard. The high PL quantum yields and the similar spectrum structures indicate that the excellent luminescence properties of DPA are maintained in TBBPA and TBNPA. The absorption and PL spectra of the TBBPA and TBNPA thin films are almost identical to those acquired in dilute CH_2Cl_2 solutions except for a slight red-shift (4 nm for TBBPA, 7 nm for TBNPA) (Fig. 2), which implies that the significant intermolecular interactions do not occur in solid thin films.

In addition, TBNPA exhibits a blue-shifted PL spectrum and a less difference between the PL spectra of the solution and thin film compared to its isomer TBDNPA (the naphthyl group is at the *para*-position of phenyl substituents in DPA).¹⁴ This can be attributed to the less conjugation length and higher non-planarity of TBNPA compared to TBDNPA (see ESI[†]).

Electrochemical properties

The electrochemical properties of TBBPA and TBNPA were investigated by cyclic voltammetry in CH₂Cl₂ containing tetrabutylammonium hexafluorophosphate (0.1 M) at a scan rate of 0.05 V s⁻¹. The electrolytic cell was a conventional three-electrode cell consisting of a Pt working electrode, a Pt wire counter electrode and an Ag/AgCl reference electrode. As shown in Fig. 3, both TBBPA and TBNPA exhibit the reversible oxidation process with almost same half-wave oxidation potentials $(E_{1/2}^{\text{ox}})$ (1.19 V for TBBPA, 1.18 V for TBNPA). The highest occupied molecular orbital (HOMO) energy levels were calculated to be -5.50 eV and -5.49 eV for TBBPA and TBNPA, respectively, by using the energy level value of -4.8 eV for



Fig. 3 Cyclic voltammograms of TBBPA and TBNPA in CH_2Cl_2 solution.

ferrocene (Fc) with respect to a zero vacuum level.^{29,30} The band gaps were determined to be 2.90 eV for TBBPA and 2.89 eV for TBNPA from the absorption band edges (Fig. 2, 427 nm for TBBPA, 429 nm for TBNPA). The lowest unoccupied molecular orbital (LUMO) energy levels were estimated to be -2.60 eV for both TBBPA and TBNPA according to the HOMO energy level values in combination with the band gaps.

Electroluminescence properties of multilayer OLEDs

To investigate the electroluminescence (EL) properties of the anthracene derivatives, we fabricated the non-doped devices, device I: ITO/NPB (30 nm)/TBBPA (30 nm)/TPBI (30 nm)/



Fig. 4 EL spectra of device I (a) and device II (b) under different luminance.



Fig. 5 Current density-voltage-luminance characteristics of the devices I and II.

LiF (2 nm)/Al, device II: ITO/NPB (30 nm)/TBNPA (30 nm)/ TPBI (30 nm)/LiF (2 nm)/Al. In these devices, ITO (indium tin oxide) and LiF/Al are the anode and the cathode, respectively; 4,4'-bis[*N*-(1-naphthyl)-*N*-phenylamino]biphenyl (NPB) is the hole transporting layer; 1,3,5-tris(*N*-phenylbenzimidazol)benzene (TPBI) is used as the electron transporting and hole blocking layer; TBBPA and TBNPA are the emitting layers (EML).

Fig. 4 shows the normalized EL spectra of the devices I and II under different luminance. It can be found that the EL spectra of devices I and II are similar to the PL spectra in dilute CH₂Cl₂ solutions and thin films, especially for TBBPA. The emission peaks of the device I based on TBBPA are at 424 nm and 448 nm, the TBNPA based device II shows an emission peak at 448 nm with a shoulder peak at 428 nm. The EL spectra of the two devices do not show an obvious red-shift compared to the PL spectra of TBBPA and TBNPA thin films, and show no emission at longer wavelength from the exciplex species. This may be attributed to the highly noncoplanar structures of TBBPA and TBNPA because of the presence of the phenyl group or naphthyl group at the orthoposition of phenyl substituents in DPA. Significantly, the EL spectra of the devices show a little change under different luminance from 10 cd m^{-2} to 1000 cd m^{-2} , which is highly desirable for OLEDs. The 1931 CIE coordinates (0.15, 0.07) of the devices are very close to the NTSC blue standard.



Fig. 6 Relative energy levels diagram of the devices based on TBBPA and TBNPA.



Fig. 7 External quantum efficiency as a function of the current density for devices I and II.

The current density-voltage-luminance characteristics of the devices I and II are shown in Fig. 5. The turn-on voltages (corresponding to 1.0 cd m^{-2}) are 3.3 V and 3.2 V for the devices I and II, respectively. The important reason for such low turn-on voltages is the small injection barriers in these devices. As shown in the relative energy levels diagram of the devices (Fig. 6), the injection barriers of both the NPB/EML interface and EML/ TPBI interface are about 0.1 eV. It is noted that, even at a practical luminance of 100 cd m⁻², the applied voltages are only 4.4 V and 4.2 V for devices I and II, respectively, and the external quantum efficiencies are 2.52% and 2.45% at this luminance. As shown in Fig. 7, device I achieves a maximum external quantum efficiency of 3.0% at 3.5 V, which is comparable to the best of the non-doped deep-blue OLEDs with a CIE coordinate of $v < 0.10^{12,14,31,32}$ Device II achieves a maximum external quantum efficiency of 2.5% at 4 V with a current density of about 6.2 mA cm⁻², meanwhile, it exhibits a lower efficiency rolloff. The high performance of devices I and II: low applied voltage, stable emission, high efficiency and the CIE coordinates matched to the NTSC blue standard, indicating that TBBPA and TBNPA are promising candidates for non-doped deep-blue OLEDs.

Conclusions

Two novel anthracene derivatives TBBPA and TBNPA are synthesized by introducing the phenyl group or naphthyl group at the *ortho*-position of phenyl substituents in DPA. Both the two anthracene derivatives have highly non-coplanar structures, and show deep-blue emission with high fluorescence quantum yields. The non-doped devices based on the two anthracene derivatives exhibit low turn-on voltage and stable deep-blue emission with high efficiency. The 1931 CIE coordinates (0.15, 0.07) of the devices are very close to the NTSC blue standard. The high performances of the devices indicate that TBBPA and TBNPA are promising candidates for non-doped deep-blue OLEDs.

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