



Simple oxadiazole derivatives as deep blue fluorescent emitter and bipolar host for organic light-emitting diodes

Yanming Wang^{a,b,*}, Haidong Huang^a, Yan Wang^a, Qun Zhu^a, Junchao Qin^a

^a School of Chemistry and Chemical Engineering, Inner Mongolia University of Science and Technology, 7 Aldine Street, Baotou, 014010, Inner Mongolia, China

^b School of Chemistry, Dalian University of Technology, 2 Linggong Road, Dalian, 116024, China

ARTICLE INFO

Keywords:

Bipolar
Oxadiazole
Color saturation
Fluorescence
Organic light emitting diodes

ABSTRACT

To obtain highly efficient and stable electroluminescence, a bipolar molecule of 2, 5-bis(4'-(9H-carbazol-9-yl)-[1,1'-biphenyl]-4-yl)-1, 3, 4-oxadiazole (Oxd-bCz) is designed and synthesized. By incorporating electron-donating and electron-withdrawing moieties into a single molecule endows the compound bipolar characteristic and obtains high performance OLED. Oxd-bCz emits purple-blue fluorescence with emission peak at 431 nm in dilute dichloromethane. The blue OLED with Oxd-bCz as emitter exhibited high performances of a low turn-on voltage of 3.6 V and a maximum external quantum efficiency of 5.6% with excellent color saturation (CIE_y ~ 0.07). With a triplet energy of 2.39eV, Oxd-bCz can be utilized as host for Ir (ppy)₃-guested green OLED with a low turn-on voltage of 2.8 V, current efficiency of 29 cd/A and an EQE value of 8.17%.

1. Introduction

Organic light emitting diodes (OLEDs) have been considered the third generation display technology after cathode-ray tube (CRT) and liquid crystal display (LCD). After decades development, OLEDs have been realized industrialization and are widely used in display fields, especially in portable electronic products [1,2]. Though organic phosphorescence and thermally activated delayed fluorescence have developed rapidly these years, the fluorescence organic emitters are still utilized most in OLED industries for the low cost, long lifetime and stable performances. Of the three primary emitters (blue, green and red) to realize full color display and white lighting, red and green emitters with long operation lifetimes and high efficiencies have been reported [3]. However, blue materials with favorable performances are rare [4]. Although various blue organic emitters containing one of the following moieties such as anthracene [5,6], fluorine [7–9], carbazole [10,11] and phenanthroimidazole [12,13] have been developed, few of them have Commission International de l'Éclairage (CIE) *y* coordinate of < 0.08 according to the Television System Committee.

One of the strategies to obtain high performance emitters is incorporating both electron-donating (donor) and electron-withdrawing (acceptor) moieties into a single molecule to facilitate both hole and electron injection and transport [14]. But such structure will produce intramolecular charge transfer (ICT) which lowers the energy of excited

state and makes emission red shift and thus it is more difficult to obtain true blue emission. We adopted oxadiazole as electron-withdrawing moiety and carbazole as the electron-donating moiety to build bipolar molecular. Comparing to triphenylamine, carbazole has weak electron-donating ability and thus can effectively reduce intramolecular charge transfer and obtain deep blue emission. The blue OLED with Oxd-bCz as emitter exhibited excellent performances of a low turn-on voltage of 3.6 V, a peak current efficiency of 2.4 cd A⁻¹, a peak power efficiency of 1.91 m W⁻¹ and a maximum external quantum efficiency of 5.6% with CIEs of (*x* = 0.16, *y* = 0.07) at voltages from 6 V to 12 V. Oxd-bCz had a triplet energy level of 2.39eV and could be utilized as bipolar host for green OLED which exhibited a moderate performance with a low turn-on voltage of 2.8 V and efficiencies of 29 cd A⁻¹ (30.31 m W⁻¹ and 8.17%).

2. Experimental section

2.1. General information

Bruker AVANCE 500 MHz spectrophotometer and 126 MHz spectrophotometer were used to record the ¹H NMR and ¹³C NMR spectra, HP1100LC/MSD MS spectrometer was used to record mass spectra. The fluorescence and UV–vis absorption spectra were measured on a PerkinElmer LS55 spectrometer and a PerkinElmer Lambda 35

* Corresponding author. School of Chemistry and Chemical Engineering, Inner Mongolia University of Science and Technology, 7 Aldine Street, Baotou, 014010, Inner Mongolia, China.

E-mail address: wymygw@163.com (Y. Wang).

<https://doi.org/10.1016/j.optmat.2018.07.015>

Received 19 April 2018; Received in revised form 10 June 2018; Accepted 5 July 2018

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spectrophotometer at room temperature, respectively, while the phosphorescence spectra were obtained on an Edinburgh FLS920 Spectrometer at 77 K in 2-MeTHF.

The cyclic voltammetry properties were studied on an electrochemical workstation (BAS100B, USA). A conventional three electrode configuration was adopted including a glass carbon working electrode, a Pt-wire counter electrode, and a saturated calomel electrode (SCE), with ferrocene as the internal standard (-5.1eV below vacuum) [15]. Upon fully deoxygenated with argon, the sample solution in dichloromethane containing 0.1 M $[\text{Bu}_4\text{N}]\text{PF}_6$ as electrolyte was scanned at a rate of 100 mV s^{-1} at room temperature. The HOMO energy level of Oxd-bCz was calculated according to the following formula:

$$E_{\text{HOMO}} = -[E_{\text{ox}}^{\text{onset}} - F_{\text{ox}}^{\text{onset}} + 5.1]\text{eV} \quad (1)$$

Density functional theory (DFT) calculations using B3LYP functional were performed with Gaussian 09. The basis set used for the C, H, N atoms was B3LYP/6-31G.

2.2. OLED fabrication and measurements

The ITO glass substrates with a sheet resistance of $30\ \Omega$ per square were first cleaned, dried, and treated by UV-ozone for 20 min, on which a 40 nm thick PEDOT:PSS film was deposited and baked at $120\ ^\circ\text{C}$ for 30 min in air. Subsequently, the substrate was transferred into a vacuum chamber to deposit the organic layers with a base pressure less than 10^{-6} Torr (1 Torr = 133.32 Pa). The evaporation rate and thickness of organic layer were monitored by a quartz oscillator. When the functional layer deposited on the glass and on the quartz oscillator, there was a decrease of hertz number on the display panel and 10 Hz was equal to 1 nm. After all the organic layers deposited on the ITO glass, a thin layer of LiF (1 nm) was thermally deposited onto organic layers to facilitate electron injection and then an Al film (200 nm) was deposited as the cathode. The emitting area of each pixel was determined by effective overlapping of two electrodes as 9 mm^2 . The performance parameters, including EL spectra, CIE coordinates, and J-V-B curves of the devices, were measured using a program-controlled PR705 photometer and a source-measure-unit Keithley 236 under ambient conditions at room temperature. The forward viewing external quantum efficiency (η_{ext}) was calculated by using the current efficiency, EL spectra, and human photopic sensitivity.

2.3. Synthesis

The chemical structures and synthetic routes of Oxd-bCz were depicted in Scheme 1. The intermediate 1 and 2 were synthesized according to the literature [16,17]. (4-(9H-carbazol-9-yl)phenyl)boronic acid (3) was used as received from commercial sources. Through Suzuki cross-coupling reactions, the target compounds Oxd-bCz was prepared at yield of 85%. Oxd-bCz has good solubility in common organic solvents, such as dichloromethane, tetrahydrofuran and ethyl acetate, so that it could be thoroughly purified by column chromatography and repeated recrystallization to reach a high purity for OLED applications. The

chemical structures were characterized by ^1H NMR, ^{13}C NMR spectroscopy, mass spectrometry, and elemental analysis.

2.3.1. Bis(4-bromobenzoyl)hydrazine (Intermediate 1)

4-bromobenzoyl chloride (8.78 g, 40 mmol) and sodium carbonate (2.12 g, 20 mmol) were dissolved in tetrahydrofuran (200 ml) in a 500 mL three-neck flask. The mixture was stirred at a room temperature. Then hydrazine hydrate (1.06 ml, 20 mmol) was dripped slowly into the solution through a 10 mL dropping funnel. The mixture was stirred at room temperature for 2 h then raised the temperature to $80\ ^\circ\text{C}$ and stirred for 10 h. After the reaction was finished, the solvents were distilled off to give a crude reaction mixture. The mixture was poured into 200 mL icy water and the precipitated solid was collected by suction filtration. Intermediate 1 was obtained as a white solid in 86% yield, and was directly used for the next step.

2.3.2. 2, 5-bis(4-bromophenyl)-1, 3, 4-oxadiazole (Intermediate 2)

A solution of bis(4-bromobenzoyl)hydrazine (6.85 g, 17.2 mmol) in thionyl chloride (50 mL) was refluxed for 12 h under N_2 atmosphere. Excess thionyl chloride was distilled off from the reaction mixture, and then the residue was slowly poured into water. Adjusting pH to 7 by saturated solution of sodium carbonate, the precipitate was suction filtrated and dried. The crude product was purified by column chromatography on silica gel with petroleum ether/dichloromethane (1:6) as the eluent to give Intermediate 2 as white solid (5.73 g, 87.6%).

^1H NMR (500 MHz, CDCl_3) δ : 8.03 (t, $J = 4.5\text{ Hz}$, 2H), 8.02 (t, $J = 4.5\text{ Hz}$, 2H), 7.72 (t, $J = 4.5\text{ Hz}$, 2H), 7.70 (t, $J = 4.5\text{ Hz}$, 2H).

^{13}C NMR (126 MHz, CDCl_3) δ : 164.05, 132.50, 128.34, 126.63, 122.62.

TOF-EI-MS (m/z): 378.9 $[\text{M} + 1]^+$.

The assignments of each proton and carbon were shown in Fig. S1 and S2 of supporting information.

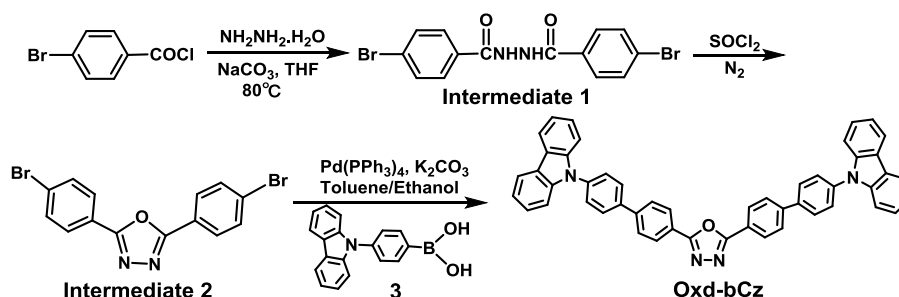
2.3.3. 2,5-bis(4'-(9H-carbazol-9-yl)-[1,1'-biphenyl]-4-yl)-1,3,4-oxadiazole

A mixture of 2,5-bis(4-bromophenyl)-1,3,4-oxadiazole (0.76 g, 20 mmol), (4-(9H-carbazol-9-yl)phenyl) boronic acid (3) (1.26 g, 44 mmol), toluene (10 mL), ethanol (2 mL), aqueous sodium carbonate (2 M, 2.5 mL), and tetrakis (triphenylphosphino) palladium (0) (0.14 g, 0.12 mmol) was refluxed at $80\ ^\circ\text{C}$ under nitrogen atmosphere overnight. After cooling and filtrating, the residue was purified by column chromatography over silica using dichloromethane/ethyl acetate (6:1) as eluent to give pure Oxd-bCz as a white solid (0.95 g, 85% yield).

^1H NMR (500 MHz, CDCl_3) δ : 8.31 (d, $J = 8.5\text{ Hz}$, 4H), 8.17 (d, $J = 8.0\text{ Hz}$, 4H), 7.90 (t, $J = 16.0\text{ Hz}$, 8H), 7.71 (d, $J = 8.5\text{ Hz}$, 4H), 7.50 (d, $J = 8.0\text{ Hz}$, 4H), 7.45 (t, $J = 15.0\text{ Hz}$, 4H), 7.32 (t, $J = 15.0\text{ Hz}$, 4H).

^{13}C NMR (126 MHz, CDCl_3) δ : 164.51, 143.53, 140.72, 138.75, 137.82, 128.62, 127.75, 127.63, 127.50, 126.06, 123.55, 123.04, 120.41, 120.17, 109.79.

TOF-EI-MS (m/z): 705.29 $[\text{M} + \text{H}]^+$. Anal. Calcd for $\text{C}_{50}\text{H}_{32}\text{N}_4\text{O}$: C 85.20, H 4.58, N 7.95. Found: C, 85.14; H, 4.63; N 7.89.



Scheme 1. Chemical Structures and Synthetic Route of Oxd-bCz.

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