

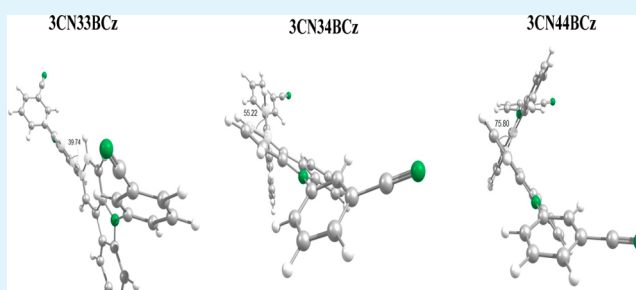
Engineering of Interconnect Position of Bicarbazole for High External Quantum Efficiency in Green and Blue Phosphorescent Organic Light-Emitting Diodes

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ABSTRACT: Three bicarbazole based host materials with different interconnect positions between carbazole units, 3,3'-(9,9'-[3,3'-bicarbazole]-9,9'-diyl)dibenzonitrile (3CN33BCz), 3,3'-(9,9'-[3,4'-bicarbazole]-9,9'-diyl)dibenzonitrile (3CN34BCz), and 3,3'-(9,9'-[4,4'-bicarbazole]-9,9'-diyl)dibenzonitrile (3CN44BCz), were developed and their synthesis, material characterization, and device characterization were reported. Two carbazole units were connected via 3,3', 3,4', and 4,4'-positions to correlate the interconnect positions with photophysical properties and device performances. The linkage via 4,4'-position increased triplet energy and thermal stability of the host materials, while the linkage via 3,3'-position enhanced current density. All bicarbazole host materials showed good device performances and high quantum efficiency above 25% was attained using the bicarbazole derivatives for green and blue phosphorescent organic light-emitting diodes. In particular, the bicarbazole host materials with a linkage via 4-position showed high quantum efficiency above 30% in the green devices.

KEYWORDS: bicarbazole, green phosphorescent device, high efficiency, benzonitrile, interconnect position



INTRODUCTION

Host materials for phosphorescent organic light-emitting diodes (PHOLEDs) play an important role of improving the device performances by managing energy transfer to dopant, charge balance, and exciton confinement. For these purposes, the host materials for PHOLEDs have been developed to possess high triplet energy, bipolar character, and appropriate energy levels. In particular, blue host materials require high triplet energy above 2.80 eV to transfer emission energy to blue triplet emitters.

There have been several classes of host materials developed to improve the device performances of PHOLEDs and representative core structure useful in PHOLEDs is bicarbazole with two carbazole units directly connected each other via C–C chemical bond.^{1–11} The bicarbazole core can allow the development of thermally stable host materials^{1–3} or hole transport materials^{4–10} because of rigidity of the core and hosts owing to high triplet energy of the bicarbazole core.

Several bicarbazole compounds have been synthesized as the host materials for PHOLEDs. Kido et al. reported four functionalized 3,3'-bicarbazole compounds as the hosts of blue PHOLEDs.¹ Several moieties such as diphenylphosphine oxide, diphenylamine, and triphenylsilane were introduced as the functional groups to modify the charge transport character of the 3,3'-bicarbazole type host materials. High quantum efficiency of 20% and low driving voltage of 3.1 V at 100 cd/m² were reported using the 3,3'-bicarbazole derivatives as the host materials. Liao et al. also reported bicarbazole derivatives as the bipolar host materials by attaching diphenylphosphine oxide or

CN as electron withdrawing moieties for bipolar charge transport properties.² High quantum efficiency of 19.3% in blue device was demonstrated using CN modified bicarbazole derivatives as the host materials. In addition, the bicarbazole derivatives were also useful as a soluble host material for solution processed devices. However, there has been no study about the bicarbazole derivatives with different interconnect positions other than 3,3'-linkage although several 3,3'-bicarbazole derivatives have been demonstrated and exhibited good device performances. Previous studies were mostly focused on correlating the electron withdrawing moieties with the device performances and basic material properties of the bicarbazole compounds.

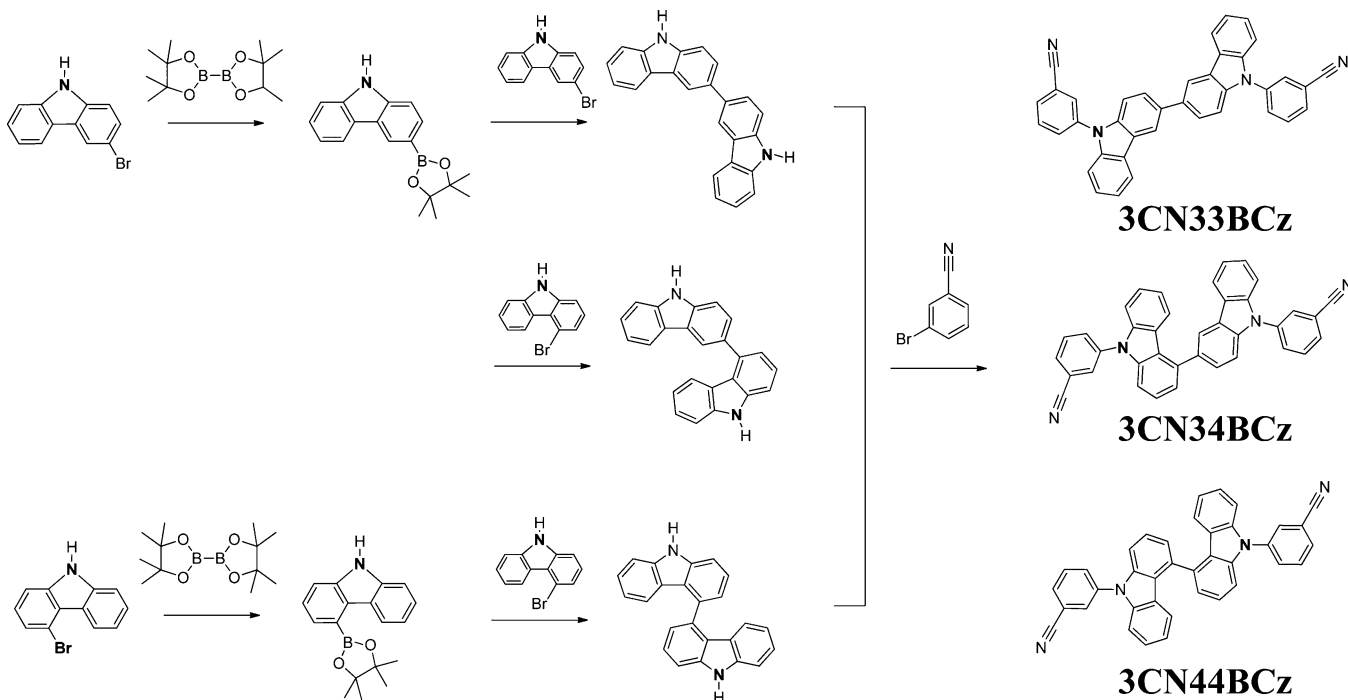
In this work, three bicarbazole derivatives with different interconnect positions, 3,3', 3,4', and 4,4', were prepared as host materials of PHOLEDs to examine the influence of interconnect position on the device output of PHOLEDs. The interconnect position was correlated with physical properties and device data of the bicarbazole type materials. It was revealed that the 4,4'-linkage increased triplet energy and thermal stability of the host materials, and the 3,3'-linkage enhanced current density. All bicarbazole materials showed good device data in the green and blue PHOLEDs and high quantum efficiency above 25% was realized using the bicarbazole derivatives as the hosts in green and blue

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Scheme 1. Synthetic Scheme of 3CN33BCz, 3CN34BCz, and 3CN44BCz



PHOLEDs. In particular, the 3,4'- and 4,4'-linkage based hosts performed well in the green PHOLEDs and the maximum quantum efficiency was above 30% in the green PHOLEDs with 3,4'- and 4,4'-linked host materials.

EXPERIMENTAL SECTION

General Information. Potassium carbonate (K_2CO_3), potassium phosphate (K_3PO_4), and 1,4-dioxane were purchased from Duksan Sci. Co. and bis(pinacolato)diboron, 3-bromo-9H-carbazole, and 1,1'-bis(diphenylphosphino)ferrocene-palladium(II)dichloride dichloromethane were products of P&H Co. Potassium acetate (CH_3CO_2K), 3-bromobenzonitrile, 4-bromobenzonitrile, copper iodide, tetrakis(triphenylphosphine) palladium(0), and (\pm)-trans-1,2-diaminocyclohexane were obtained from Aldrich. Co. and all reactants were used as received.

Synthesis. Synthetic scheme of 3CN33BCz, 3CN34BCz, and 3CN44BCz compounds is described in Scheme 1.

9H,9'H-3,3'-bicarbazole. A solution of 3-bromo-9H-carbazole (1.5 g, 6.1 mmol), 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (2.32 g, 7.9 mmol) and tetrakis(triphenylphosphine)-palladium(0) (0.21 g, 0.2 mmol) were put in round bottomed flask filled with in tetrahydrofuran (60 mL) and K_2CO_3 (8.29 g, 2M) in water (30 mL) was added. After reflux for 24 h and cooling to room temperature, extraction using methylene chloride and water was carried out. The organic layer was dehydrated using $MgSO_4$ and solvent was removed to obtain a product after filtering of $MgSO_4$. The product was purified by column chromatography using ethyl acetate: *n*-hexane (1:4) (1.2 g, yield 59%). 1H NMR (400 MHz, DMSO): δ 11.26 (s, 2H), 8.50 (s, 2H), 8.25–8.22(m, 2H), 7.82–7.79 (m, 2H), 7.59–7.37 (m, 6H), 7.21–7.16 (m, 2H). MS (FAB) m/z 332[(M+H) $^+$].

3,3'-(9H,9'H-[3,3'-bicarbazole]-9,9'-diyl)dibenzonitrile (3CN33BCz). A solution of 9H,9'H-3,3'-bicarbazole (1.5 g, 4.5 mmol), 3-bromobenzonitrile (2.05 g, 11.3 mmol), copper iodide (0.52 g, 2.7 mmol), and K_3PO_4 (2.49 g, 18.1 mmol) in 1,4-dioxane (40 mL) was prepared and (\pm)-trans-1,2-diaminocyclohexane (0.31 g, 2.7 mmol) was added. The solution was refluxed for 48 h and extracted with ethyl acetate and water. Other processes were the same as the synthesis of 9H,9'H-3,3'-bicarbazole. White powder was collected as a product (1.3 g, yield 54%). 1H NMR (400 MHz, $CDCl_3$): δ 8.45 (s,

2H), 8.24 (d, 2H, J = 8.0 Hz), 7.96–7.89(m, 4H), 7.81–7.70(m, 6H), 7.50–7.35 (m, 8H). ^{13}C NMR (400 MHz, $CDCl_3$): δ 140.8, 139.6, 139.1, 135.0, 131.5, 131.1, 130.9, 130.4, 126.6, 126.2, 124.5, 124.0, 121.0, 120.8, 119.3, 118.0, 114.4, 109.7, 109.5. MS (FAB) m/z 534[(M+H) $^+$]. Anal. calcd for $C_{38}H_{22}N_4$: C, 85.37; H, 4.15; N, 10.48. Found: C, 84.69; H, 3.92; N, 10.52.

9H,9'H-3,4'-bicarbazole. Synthesis of 9H,9'H-3,4'-bicarbazole was carried out according to the method for the synthesis of 9H,9'H-3,4'-bicarbazole except that 4-bromo-9H-carbazole was used instead of 3-bromo-9H-carbazole (0.9 g, yield 44%). 1H NMR (400 MHz, $CDCl_3$): δ 8.33 (s, 1H), 8.13 (s, 2H), 8.06 (d, 1H, J = 8.0 Hz), 7.70 (d, 1H, J = 8.0 Hz), 7.58 (d, 1H, J = 8.0 Hz), 7.52–7.42 (m, 6H), 7.33 (t, 1H, J = 16.0 Hz), 7.24–7.21 (m, 2H), 6.88 (t, 1H, J = 16.0 Hz). MS (FAB) m/z 332 [(M+H) $^+$].

3,3'-(9H,9'H-[3,4'-bicarbazole]-9,9'-diyl)dibenzonitrile (3CN34BCz). Synthetic procedure of 3CN34BCz was the same as that of 3CN33BCz. 9H,9'H-3,4'-bicarbazole was used instead of 9H,9'H-3,3'-bicarbazole (1.0 g, yield 62%). 1H NMR (400 MHz, $CDCl_3$): δ 8.41 (s, 1H), 8.14(d, 1H, J = 8.0 Hz), 8.03–7.88(m, 4H), 7.81–7.72 (m, 5H), 7.57–7.45(m, 5H), 7.38–7.30(m, 5H), 7.01(s, 1H). ^{13}C NMR (400 MHz, $CDCl_3$): δ 140.9, 140.8, 140.0, 139.0, 138.5, 133.7, 132.1, 131.6, 131.2, 131.0, 130.5, 127.8, 126.7, 126.2, 124.1, 124.0, 123.6, 123.0, 122.7, 121.6, 121.2, 121.1, 120.8, 120.5, 118.0, 114.4, 109.6, 109.4, 109.1, 108.1. MS (FAB) m/z 534 [(M+H) $^+$]. Anal. calcd for $C_{38}H_{22}N_4$: C, 85.37; H, 4.15; N, 10.48. Found: C, 85.40; H, 4.30; N, 10.28.

9H,9'H-4,4'-bicarbazole. Synthetic method of 9H,9'H-4,4'-bicarbazole was the same as that of 9H,9'H-3,4'-bicarbazole. 4-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole was a reactant instead of 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole (0.9 g, yield 44%). 1H NMR (400 MHz, DMSO): δ 11.43(s, 2H), 7.66–7.62 (m, 2H), 7.58–7.53 (m, 2H), 7.44–7.40 (m, 2H), 7.20–7.12 (m, 4H), 6.63–6.49 (m, 4H). MS (FAB) m/z 332[(M+H) $^+$].

3,3'-(9H,9'H-[4,4'-bicarbazole]-9,9'-diyl)dibenzonitrile (3CN44BCz). 3CN44BCz was synthesized according to the method for the synthesis of 3CN33BCz. 9H,9'H-4,4'-bicarbazole was starting material instead of 9H,9'H-3,3'-bicarbazole (2.1 g, yield 87%). 1H NMR (400 MHz, $CDCl_3$): δ 8.02 (s, 2H), 7.99–7.96 (m, 2H), 7.82–7.80 (m, 4H), 7.60 (t, 2H, J = 16.0 Hz), 7.53(d, 2H, J = 8.0 Hz), 7.42 (d, 2H, J = 8.0 Hz), 7.34–7.28 (m, 4H), 6.94 (d, 2H, J = 8 Hz), 6.87

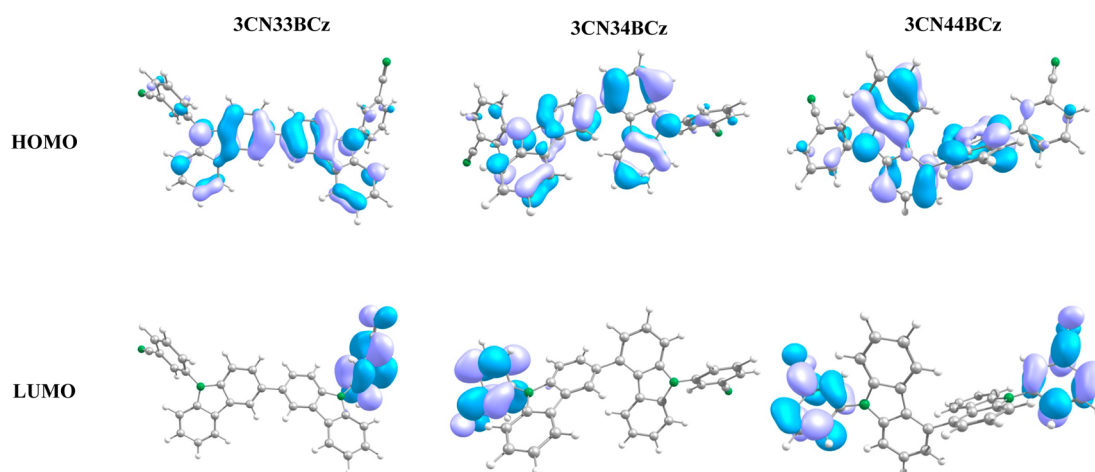


Figure 1. HOMO and LUMO distribution of 3CN33BCz, 3CN34BCz, and 3CN44BCz.

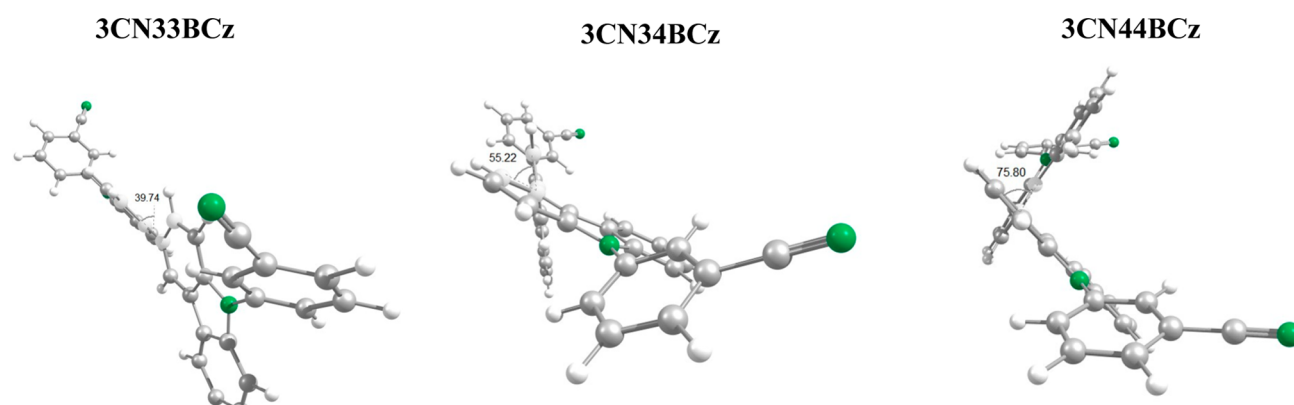


Figure 2. Geometrical structure of 3CN33BCz, 3CN34BCz, and 3CN44BCz.

(t , 2H, $J = 16.0$ Hz). ^{13}C NMR (400 MHz, CDCl_3): δ 140.9, 140.6, 139.0, 135.8, 132.0, 131.1, 131.0, 126.3, 126.2, 123.5, 122.6, 122.3, 121.9, 120.6, 118.0, 114.4, 109.0, 108.8. MS (FAB) m/z 534 [($M + \text{H}$) $^+$]. Anal. calcd for $\text{C}_{38}\text{H}_{22}\text{N}_4$: C, 85.37; H, 4.15; N, 10.48. Found: C, 85.08; H, 4.32; N, 10.16.

Device Growth and Characterization. A device configuration used to fabricate PHOLEDs was indium tin oxide (ITO, 120 nm)/poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS, 60 nm)/4,4'-cyclohexylidenebis[*N,N*-bis(4-methylphenyl)aniline] (TAPC, 20 nm)/1,3-bis(*N*-carbazolyl)benzene (mCP, 10 nm)/3CN33BCz:dopant or 3CN34BCz:dopant or 3CN44BCz:dopant (25 nm, 5% doping)/diphenylphosphine oxide-4-(triphenylsilyl)phenyl (TSPO1, 35 nm)/LiF (1 nm)/Al (200 nm). Tris(2-phenylpyridine) iridium ($\text{Ir}(\text{ppy})_3$) and iridium(III) bis((3,5-difluorophenyl)pyridine) picolate (FIrpic) were triplet emitters in the green and blue PHOLEDs, respectively. The device structure of hole only device was ITO (120 nm)/PEDOT:PSS (60 nm)/TAPC (20 nm)/mCP (10 nm)/3CN33BCz or 3CN34BCz or 3CN44BCz (25 nm)/TAPC (10 nm)/Al and the device structure of electron only device was ITO (120 nm)/Ca (10 nm)/3CN33BCz or 3CN34BCz or 3CN44BCz (25 nm)/TSPO1 (35 nm)/LiF (1 nm)/Al (100 nm). All devices were grown by vacuum evaporation process and were protected from oxygen and moisture by encapsulation. Device performance measurement, general chemical and physical analysis of the bicarbazole compounds are described in our previous work.¹²

RESULTS AND DISCUSSION

Carbazole has been generally modified at 3-position because direct halogenation of carbazole can produce a halogenated carbazole at 3-position.^{13–16} The 3-position substitution is advantageous in that high triplet energy is realized via meta

linkage among aromatic units and the highest occupied molecular orbital (HOMO) of the carbazole compound is managed by proper selection of the substituents. Compared to the 3-position substitution, 4-position substitution is rather difficult because direct halogenation cannot yield the halogenated carbazole at 4-position. The 4-position halogenated carbazole can be synthesized by ring-closing reaction of a halogenated intermediate as reported in other works.¹⁷ The 4-position substitution has a merit of thermal stability owing to steric hindrance of the substituent and high quantum efficiency due to balanced charge transport properties. However, it is still not clear how the interconnect position via C–C bond between two carbazole units will affect the physical properties and device data of bicarbazole derivatives. Therefore, three bicarbazole derivatives, 3CN33BCz, 3CN34BCz, and 3CN44BCz, were developed.

The three bicarbazole type host materials were designed to have different interconnect positions and bipolar carrier transport character. Two carbazole units were connected via 3,3', 3,4', and 4,4'-positions to examine the influence of interconnect position and 3-cyanophenyl moiety was introduced for bipolar carrier transport by improving electron transport properties. Synthetic scheme is shown in Scheme 1 and the bicarbazole compounds were synthesized by coupling two carbazole units followed by substitution of 3-cyanophenyl moiety at nitrogen of carbazole. Synthetic yields of 3CN33BCz, 3CN34BCz, and 3CN44BCz were 54%, 62%, and 87%, respectively.

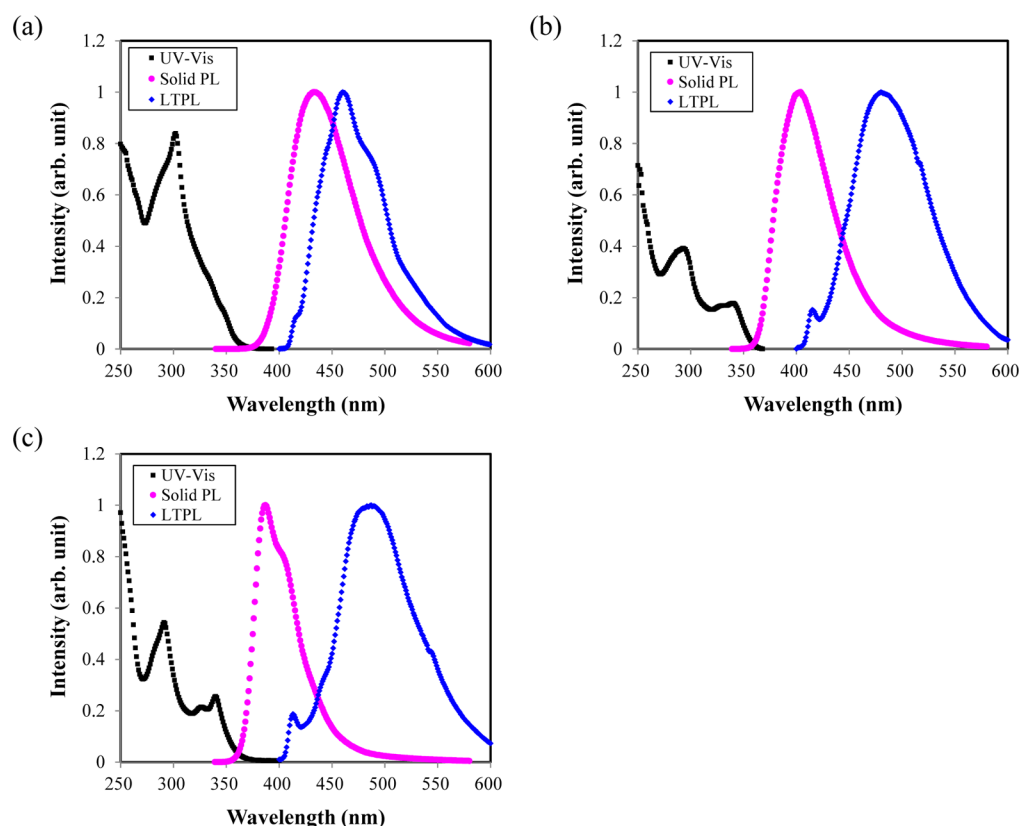


Figure 3. UV-vis, solid PL and low temperature PL spectra of 3CN33BCz (a), 3CN34BCz (b), and 3CN44BCz (c).

Molecular orbital distribution study of the bicarbazole compounds was carried out with Gaussian 09 program using B3LYP with 6-31G* basis sets. Figure 1 shows molecular orbital of 3CN33BCz, 3CN34BCz, and 3CN44BCz compounds. The HOMO of the bicarbazole compounds were distributed over the bicarbazole moiety due to high electron density in the bicarbazole by electron donating character of nitrogen of carbazole. The lowest unoccupied molecular orbital (LUMO) was dispersed over the benzonitrile unit in all bicarbazole derivatives owing to strong electron withdrawing CN unit. Donor-acceptor molecular structure of the bicarbazole compounds separated the HOMO and LUMO.

The geometrical structure of the bicarbazole compounds was also studied to correlate the interconnect position with dihedral angle at the interconnect position. Figure 2 shows geometrical structure of the bicarbazole compounds. Dihedral angles between two carbazole units of 3CN33BCz, 3CN34BCz, and 3CN44BCz were 40°, 55°, and 76°. The dihedral angle was increased by linking two carbazole units via 4-position of carbazole. Steric hindrance caused by the 4-substituted carbazole distorted the molecular structure, resulting in the large dihedral angle in the 3CN44BCz. From this result, it can be presumed that the linkage via 4-position of carbazole may help amorphous film formation and molecular rigidity.

Ultraviolet-visible (UV-vis) and photoluminescence (PL) measurements of the host materials were carried out and Figure 3 shows UV-vis, solid PL and low temperature PL spectra of 3CN33BCz, 3CN34BCz, and 3CN44BCz host materials. UV-vis absorption of the bicarbazole compounds was similar. Intense π - π^* absorption by the bicarbazole backbone structure was observed below 300 nm and weak n - π^* absorption by the bicarbazole backbone structure was detected above 300 nm.

Solid PL emission of the compounds appeared at different wavelengths depending on the interconnect position of the bicarbazole moiety. 3CN33BCz showed solid PL emission at 433 nm and the PL emission was shifted to 404 and 387 nm in 3CN34BCz and 3CN44BCz, respectively. The interconnection via 4-position of carbazole induced the blue shift of the PL emission because phenyl unit is linked through ortho-position compared to meta-position in the interconnection via 3-position. The 4-position interconnection limits the degree of conjugation due to large dihedral angle, which blue-shifted the PL emission. Similar tendency was detected in the phosphorescence PL spectra measured at low temperature and the triplet energy was in the order of 3CN33BCz (2.95 eV) < 3CN34BCz (2.98 eV) < 3CN44BCz (3.00 eV). Therefore, the linkage via 4-position of carbazole was useful to shift the PL emission to high energy and to increase the triplet energy.

The oxidation and reduction potentials of the bicarbazole compounds were analyzed using cyclic voltammetry (CV) (Figure 4). The order of oxidation and reduction potentials of the bicarbazole compounds were 3CN44BCz > 3CN34BCz > 3CN33BCz. The linkage via 4-position shifted the oxidation and reduction potentials to high voltage. Ionization potentials (IPs) of the 3CN33BCz, 3CN34BCz, and 3CN44BCz calculated from the oxidation potential were -5.90 eV, -6.11 eV, and -6.24 eV, respectively. Electron affinities (EAs) from the reduction potentials were -2.89 eV, -2.98 eV, and -3.07 eV for 3CN33BCz, 3CN34BCz, and 3CN44BCz, respectively. The energy gaps between IPs and EAs were 3.01, 3.13, and 3.17 eV for 3CN33BCz, 3CN34BCz, and 3CN44BCz, respectively. The introduction of 4-linkage in the bicarbazole compounds increased the IP-EA gap, which agrees with the PL data of the three compounds. As shown in Figure 2, the dihedral angle

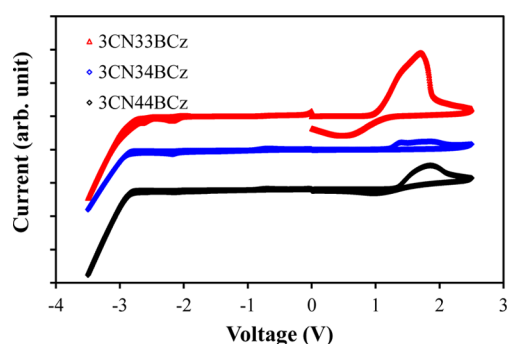


Figure 4. CV curves of 3CN33BCz, 3CN34BCz, and 3CN44BCz.

between two carbazole units was high in the 3CN34BCz and 3CN44BCz materials with a linkage via 4-position. The large dihedral angle suppressed the degree of conjugation and increased the IP–EA gap of 3CN34BCz and 3CN44BCz.

Thermal properties of the host materials were analyzed using differential scanning calorimeter (DSC). DSC curves of the bicarbazole compounds are shown in Figure 5. Glass transition

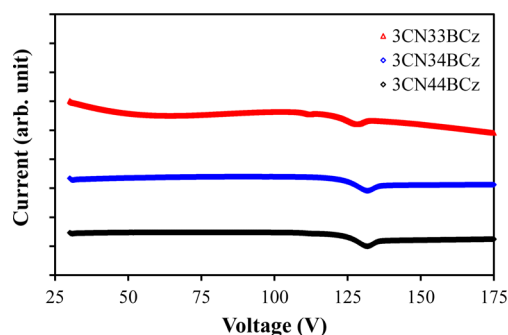


Figure 5. DSC curves of 3CN33BCz, 3CN34BCz, and 3CN44BCz.

temperatures from the DSC curves were 128, 132, and 132 °C for 3CN33BCz, 3CN34BCz, and 3CN44BCz, respectively. 3CN34BCz and 3CN44BCz with a linkage via 4-position showed high glass transition temperature due to rigidity of the molecular structure as reported in other work.¹⁷

Thermal stability of the bicarbazole compounds was further studied by analyzing the morphological change of the vacuum evaporated film. Figure 6 shows optical microscopic pictures of vacuum evaporated film of the host materials at 110 and 120 °C after 10 min annealing at the measurement temperatures. There was no morphological change of all films at 110 °C, but the uniform morphology of 3CN33BCz was disrupted at 120 °C, which confirms that the linkage via 4-position improved thermal stability of the bicarbazole compounds. Compared with dihedral angles of 55° and 76° of 3CN34BCz and 3CN44BCz, the small dihedral angle of 3CN33BCz facilitated the morphological change of 3CN33BCz due to facile molecular packing, leading to relatively poor thermal stability of 3CN33BCz.

Single carrier devices were prepared to examine charge density of the bicarbazole derivatives. Figure 7 shows current density–voltage plots of single carrier devices of the host materials. The order of hole current density was 3CN34BCz > 3CN33BCz > 3CN44BCz, while the order of electron current density was 3CN33BCz > 3CN34BCz > 3CN44BCz. The interconnection via 3-position was effective to increase the current densities considering that 3CN33BCz and 3CN34BCz

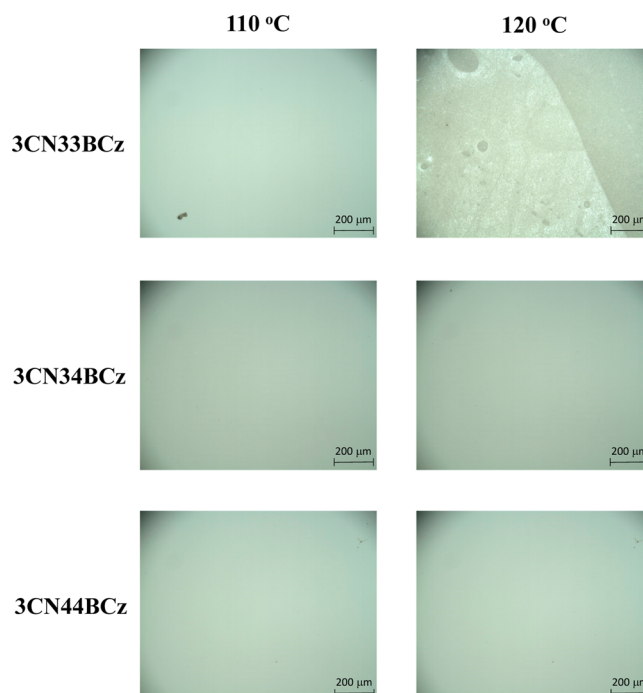


Figure 6. Optical microscopic pictures of 3CN33BCz, 3CN34BCz, and 3CN44BCz at 110 and 120 °C after thermal annealing for 10 min at the measurement temperature.

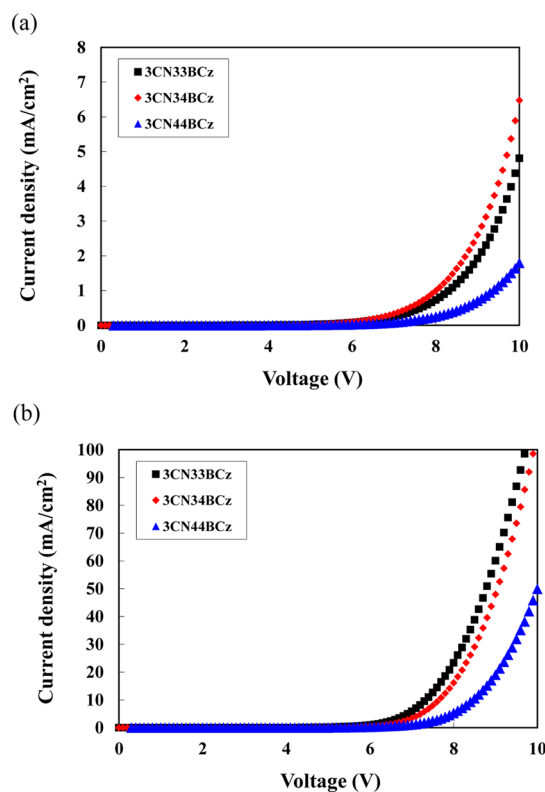


Figure 7. Current density–voltage curves of hole only devices (a) and electron only devices (b) of 3CN33BCz, 3CN34BCz, and 3CN44BCz.

showed higher current density than 3CN44BCz. As the same carbazole and benzonitrile units were used as the hole and electron transport moieties, it can be assumed that hole and electron transport properties of the subunit would be similar. Therefore, the different current densities of the bicarbazole

compounds are caused by the different geometrical structure depending on the interconnect position. 3CN33BCz and 3CN34BCz have smaller dihedral angle between two carbazole units, which facilitates charge transport due to facile molecular packing. Therefore, the current densities of the bicarbazole compounds could be explained by the dihedral angle between two carbazole units.

The bicarbazole compounds were applied as the triplet host materials for green PHOLEDs to investigate the influence of interconnect position on the device data of PHOLEDs. Current density–voltage–luminance plots of the green PHOLEDs having the bicarbazole compounds are shown in Figure 8. The

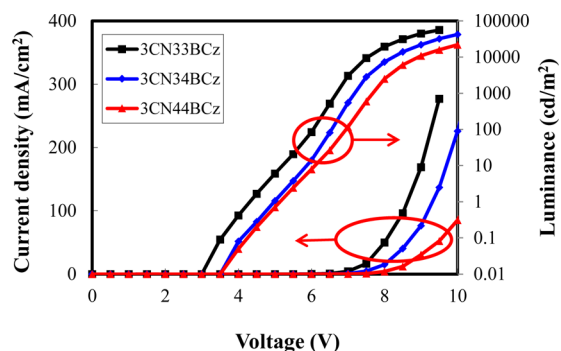


Figure 8. Current density–voltage–luminance curves of green PHOLEDs with different host materials.

order of the current density was 3CN33BCz > 3CN34BCz > 3CN44BCz, which agreed with the order of single carrier current densities of the bicarbazole compounds. In spite of lower hole current density of 3CN33BCz than electron current density of 3CN34BCz, high electron current density of 3CN33BCz induced the increase of current density of the 3CN33BCz devices. The luminance showed the same trend.

External quantum efficiency of the green PHOLEDs was plotted against luminance (Figure 9). The quantum efficiency

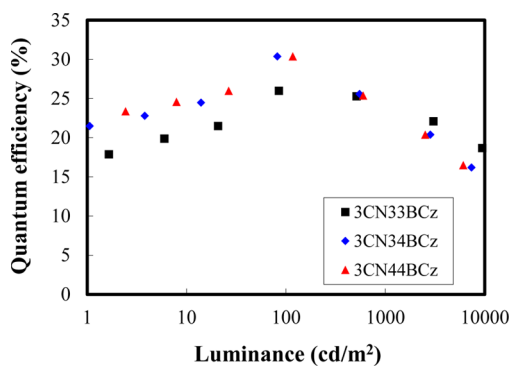


Figure 9. Quantum efficiency–luminance curves of green PHOLEDs with different host materials.

of the green PHOLEDs was high in the 3CN34BCz and 3CN44BCz devices and maximum quantum efficiencies of the 3CN34BCz and 3CN44BCz devices were 30.4% and 30.4%, respectively, compared with 26.0% of the 3CN33BCz device. The relatively higher quantum efficiency of the 3CN34BCz and 3CN44BCz devices than that of the 3CN33BCz device can be described by balanced carrier density of the devices. The comparison of current densities of the single carrier devices revealed that electrons are rich in all devices. In the case of

3CN33BCz, the ratio of electron current density to hole current density was above 20:1, while it was less than 10:1 in the 3CN34BCz and 3CN44BCz. Therefore, better charge balance can be expected in the 3CN34BCz and 3CN44BCz devices, which results in high quantum efficiency in the 3CN34BCz and 3CN44BCz devices. Overall, high quantum efficiency above 25% was obtained in the green PHOLEDs with the bicarbazole type host materials due to charge confinement, triplet exciton confinement, and good energy transfer. As described in the electroluminescence (EL) spectra in Figure 10, pure emission of only Ir(ppy)₃ was detected in the EL spectra.

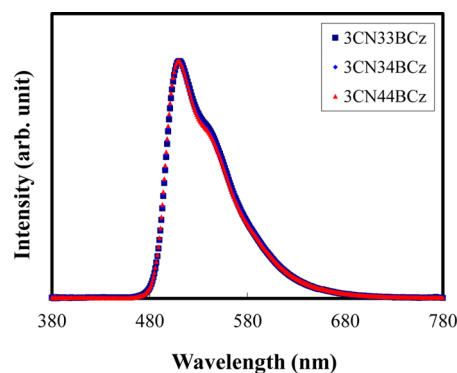


Figure 10. EL spectra of green PHOLEDs with different host materials.

Blue PHOLEDs were also grown with the bicarbazole compounds because of high triplet energy of the bicarbazole derivatives. Quantum efficiency–luminance data of the blue PHOLEDs are presented in Figure 11. All host materials

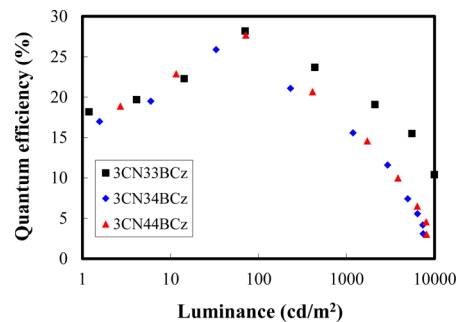


Figure 11. Quantum efficiency–luminance curves of blue PHOLEDs with different host materials.

provided high quantum efficiency above 25% in blue PHOLEDs. Therefore, the bicarbazole type host materials were effective as the triplet hosts for both green and blue PHOLEDs. Driving voltage, current density, and efficiency data are summarized in Table 1.

Comparing all photophysical and device data of the bicarbazole compounds in green PHOLEDs, 3CN34BCz showed merits of 3-position connection such as high current density and advantages of 4-position connection such as thermal stability. Therefore, interconnection via 3,4'-position was an useful way of upgrading the device performances of the bicarbazole compounds.

Table 1. Device Performances of Blue Phosphorescent Organic Light-Emitting Diodes

devices	voltage (V)	current density (mA/cm ²)	quantum efficiency (%)	current efficiency (cd/A)	power efficiency (lm/W)
	turn-on ^a 1000 cd/m ²	1000 cd/m ²	max 1000 cd/m ²	max 1000 cd/m ²	max 1000 cd/m ²
3CN33BCz (green)	3.5	1.4	26.0	80.2	46.4
	6.6		24.7	76.3	40.2
3CN34BCz (green)	4.0	1.5	30.4	93.6	50.0
	7.1		24.6	75.6	37.1
3CN44BCz (green)	4.0	1.4	30.4	93.2	46.2
	7.6		24.4	74.8	34.3
3CN33BCz (blue)	4.0	2.8	28.2	49.6	26.5
	7.2		22.1	38.9	18.9
3CN34BCz (blue)	4.5	3.6	25.9	44.7	23.9
	7.4		16.7	28.9	13.6
3CN44BCz (blue)	5.0	3.6	27.7	47.5	23.6
	7.7		18.0	31.1	14.1

^aVoltage at 0.1 cd/m².

CONCLUSIONS

In conclusion, bicarbazole type host materials with different interconnect positions, 3,3', 3,4', and 4,4', were synthesized and the interconnect position could be correlated with material parameters and device data of the bicarbazole compounds. The linkage via 4-position of carbazole increased the dihedral angle between two carbazole units, which increased the IP-EA gap and triplet energy of the host materials, and reduced current density of the devices. All bicarbazole compounds were efficient as the host materials of PHOLEDs. The bicarbazole host materials realized high quantum efficiency above 25% in blue and 30% in green PHOLEDs.

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Notes

The authors declare no competing financial interest.

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