Supporting Information

Dibenzo[c,g]indolo[3,2,1-jk]carbazole as a new chromophore for

blue organic light-emitting diodes

Vilas Venunath Patil, Kyung Hyung Lee and Jun Yeob Lee

School of Chemical Engineering, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon,

Gyeonggi 440-746, Korea

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Email: <u>leej17@skku.edu</u>

Experimental section

General information

All the reagents and solvents were procured from the commercial sources and used without further purification. The chromatographic separations were performed using silica gel (200-300 nm). The purification of all the compounds was done by column chromatography and for the final products further purification was done by temperature gradient vacuum sublimation process. The final products were confirmed by ¹H, ¹³C NMR, and MS spectrometry. The ¹H and ¹³C NMR data of the final products were recorded on JEOL 500 MHz spectrometer by using deuterated chloroform (CDCl₃) and deuterated dimethyl sulfoxide (DMSO-D6) as a solvent and chemical shift is expressed in parts per million (ppm), with tetramethylsilane (TMS) as an internal standard. The information about instrumental tools used such as cyclic-voltammetry (CV), UV-Visible absorption spectroscopy, fluorescence spectroscopy, mass spectroscopy, TGA analysis and theoretical computational were listed in our previous work.^[1]

Synthetic procedures

Synthesis of 7H-dibenzo[c,g]carbazole (1a)

The synthesis of **1a** was carried out by modifying the literature reported process.^[2] A mixture of [1,1'-binaphthalene]-2,2'-diamine (1 g, 3.52 mmol, 1 equiv.), conc. hydrochloric acid (HCl) (7 mL), and 1,4-dioxane (90 mL) were refluxed in a sealed tube for 24 h. The reaction mixture was neutralized by 5% sodium bicarbonate solution and extracted using dichloromethane three times. The organic layer was washed with water three times and dried over anhydrous magnesium sulfate (MgSO₄). The crude product obtained after evaporating the solvent was

purified by column chromatography (Hexane: dichloromethane - 80:20) to give **1a**. White-colored solid; Yield: 0.54 g (57%); MS- calcd. for $C_{20}H_{13}N$ - 267.33; found- 268.59.

Synthesis of 7-(2-bromophenyl)-7*H*-dibenzo[c,g]carbazole (2a)

A mixture of **1a** (2 g, 7.48 mmol, 1 equiv.), 1-bromo-2-fluorobenzene (8.5 g, 29.92 mmol, 4 equiv.), and cesium carbonate (Cs_2CO_3) (9.8 g, 29.92 mmol, 4 equiv.) was refluxed in 50 mL of *N*, *N* dimethylformamide (DMF) for 6 h. The reaction progress was monitored by thin-layer chromatography (TLC). The reaction mass was poured in 500 mL of water and stirred for 2 h and then extracted using dichloromethane three times. The organic layer was washed with water, dried on anhydrous MgSO₄. The solvent was evaporated under vacuum and the crude product obtained was purified by column chromatography (Hexane: dichloromethane 95:5) to give **2a**. White-colored solid; Yield: 4.8 g (76%); MS- calcd. for C₂₆H₁₆BrN- 422.32; found- 423.13.

Synthesis of dibenzo[c,g]indolo[3,2,1-jk]carbazole (DBICz-core) (3a)^[3]

A mixture of **2a** (2.4 g, 5.68 mmol, 1 equiv.), palladium (II) acetate $[Pd(OAc)_2]$ (0.18 g, 0.8 mmol, 0.14 equiv.), triphenylphosphine (PPh₃) (0.52 g, 1.98 mmol, 0.35 equiv.), benzyl triethyl ammonium chloride (1. 29 g, 5.68 mmol, 1 equiv.), and potassium carbonate (K₂CO₃) (3.93 g, 28.41 mmol, 5 equiv.) was refluxed in *N*, *N* dimethylacetamide (DMAc) (50 mL) for 6 h. The reaction mass poured in 500 mL of water and extracted in dichloromethane. The reaction mass washed with water three times and dried on anhydrous MgSO₄. The crude product obtained after evaporating the solvent was further purified by using column chromatography (100% hexane) to give **3a**. White colored solid; Yield: 1.0 g (52%); ¹H NMR (500 MHz, CDCl₃) δ 9.27 (dd, *J* = 8.5, 3.5 Hz, 2H), 8.43 (s, 1H), 8.30 (d, *J* = 8.1 Hz, 1H), 8.16 (d, *J* = 7.6 Hz, 1H), 8.11 (d, *J* = 8.7 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.95 (dd, *J* = 18.8, 8.3 Hz, 2H), 7.81 (dt, *J* = 19.1, 7.6 Hz, 2H), 7.58

(dt, J = 16.0, 7.6 Hz, 3H), 7.37 (t, J = 7.5 Hz, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 141.72 (s), 140.63 (s), 134.62 (s), 133.56 (s), 131.90 (s), 130.57 (s), 130.40 (s), 130.15 (s), 129.64 (s), 129.43 (s), 128.23 (s), 127.43 (s), 126.59 (d, J = 16.8 Hz), 126.05 (s), 125.83 (s), 125.12 (s), 123.91 (d, J = 10.8 Hz), 123.23 (s), 122.78 (s), 121.04 (s), 120.50 - 120.35 (m), 113.14 (s), 112.42 (s); MS-calcd. for C₂₆H₁₅N- 341.41; found- 342.39.

Synthesis of 14-bromodibenzo[c,g]indolo[3,2,1-jk]carbazole (4a)^[4]

To a solution of **3a** (0.5 g, 1.47 mmol, 1 equiv.) in 10 mL of dichloromethane was added *N*-bromosuccinimide (NBS) (0.26 g, 1.47 mmol, 1 equiv.) in 2 mL of DMF slowly at room temperature. The reaction was stirred at room temperature for 12 h and the progress of the reaction was monitored by TLC. The reaction mass was poured in 100 mL of water and the crude product was extracted using dichloromethane. The organic layer was dried over MgSO₄ and purified by column chromatography (100% hexane) to give **4a**. White-colored solid; Yield: 0.5 g (81%); MS-calcd. for C₂₆H₁₄BrN- 420.31; found- 423.76.

N,*N*-diphenyldibenzo[c,g]indolo[3,2,1-*jk*]carbazol-14-amine (DBICz-DPA)

A mixture of 4a (0.25 g, 0.6 mmol, 1 equiv.), diphenylamine (0.12 g, 0.7 mmol, 1.2 equiv.), sodium tert. butoxide (0.12 g, 1.2 mmol, 2 equiv.) in 20 mL of xylene was stirred for 10 min at atmosphere. room temperature under nitrogen А mixture of а bis(dibenzylideneacetone)palladium(0) [Pd(dba)₂] (0.034 g, 0.06 mmol, 0.1 equiv.), tri-tertbutylphosphine [P(t-Bu)₃] (0.024, 0.12 mmol, 02 equiv.) in xylene (10 mL) was added slowly at room temperature. The reaction mass was heated to reflux for 24 h and the progress of the reaction was monitored by TLC. The reaction mass was cooled to room temperature and diluted with dichloromethane (50 mL). The insoluble residue was removed by filtration through the celite bed. The organic layer was evaporated under vacuum and purified by using column chromatography (Hexane:dichloromethane-80:20) to give **DBICz-DPA**. Yellow colored solid, 0.19 g (63%); 1H NMR (500 MHz, CDCl3) δ 9.37 (dd, J = 30.0, 8.5 Hz, 2H), 8.57 – 8.50 (m, 4H), 8.35 (d, J = 8.1 Hz, 3H), 8.23 (dd, J = 28.1, 7.9 Hz, 7H), 8.11 – 7.97 (m, 6H), 7.83 (ddd, J = 22.3, 15.0, 7.4 Hz, 12H), 7.73 – 7.34 (m, 18H), 7.25 (dd, J = 9.8, 6.0 Hz, 19H), 7.21 – 7.14 (m, 16H), 6.95 (dt, J = 28.4, 7.1 Hz, 8H). ¹³C NMR (126 MHz, CDCl₃) δ 148.54 (s), 147.45 – 147.29 (m), 142.57 (s), 140.71 – 140.55 (m), 134.88 (s), 133.77 (s), 132.01 (s), 131.79 (s), 130.18 (s), 129.64 – 129.23 (m), 128.34 (d, *J* = 14.8 Hz), 126.89 (d, *J* = 18.9 Hz), 126.61 (s), 125.94 (d, *J* = 13.2 Hz), 124.67 (s), 124.10 (s), 123.90 (s), 123.44 (s), 122.99 (s), 122.02 (d, *J* = 12.9 Hz), 121.16 (d, *J* = 12.1 Hz), 120.54 (s), 115.03 (s), 113.14 (s), 112.65 (s); MS- calcd. for C₃₈H₂₄N₂- 508.62; found- 509.47.

Device fabrication and measurement

The OLED devices were fabricated by using a transparent glass substrate with 50 nm thick indium tin oxide (ITO). The cleaning of the ITO glass substrate was done using acetone and deionized water by ultrasonic treatment. The deposition of all the layers was carried out by vacuum thermal evaporation under the pressure of 3.0 x 10-7 torr. The deposition rates for the organic layers, LiF, and Al were controlled at 0.1, 0.01, and 0.5 nm/s, respectively. The sky-blue device structure was ITO (50 nm), BPBPA:HATCN (40 nm: 30%)/ BPBPA (10 nm)/ LBIL001 (10 nm)/ PANB: emitter (5%) (30 nm)/ TNPT (5 nm)/ ZADN (20 nm)/ LiF (1.5 nm)/ Al (200 nm). The encapsulation on glass was performed under the inert atmosphere (N2 atmosphere) to protect the device from O2. All the device measurements were performed at ambient temperature. The electrical and optical characterizations of the devices were carried out by using Keithley 2400 Source Meter and CS 2000 spectroradiometer, respectively.



Fig. S1 Optimized structures and HOMO-LUMO distribution of **DBICz**-core and **DBICz-DPA** by using **B3LYP/6-311+G**** basic sets of Gaussian 09 software



Fig. S2 UV-vis (dilute THF solution), solution (dilute THF solution), and Film PL (**DBICz** doped at 3 wt% concentration PS film) curves of **DBICz** chromophore



Fig. S3 TGA curve of DBICz-DPA



Fig. S4 Schematic device diagram



Fig. S5 Luminance V/s current efficiency curves for A, B, and C devices



Fig. S6 The luminous pictures of A, B, and C devices at 1000 cd/m^2

λ_{abs}	λ_{abs} $\lambda_{PL}(nm)$		PLQY	Ese	HOMO ^f	LUMO ^g	Egh	Tdi
(nm) ^a	Solution ^a	film ^b	(%)	(eV)	(eV)	(eV)	(eV)	(⁰ C)
240, 249, 279, 331, 405	477	469	94.1°/92.3d	3.11	-5.68	-2.73	2.95	408.2

Table S1. Photophysical, electrochemical and thermal analysis data of DBICz-DPA

^aMeasured in toluene solution at room temperature. ^bMeasured in emitter 3 wt% doped PANB film. ^cUnder nitrogen. ^dUnder air. ^eEstimated from the onset value of solid PL spectra at room temperature. ^fMeasured by cyclic voltammetry. ^gCalculated by subtracting HOMO and optical bandgap. ^hOptical bandgap. ⁱDecomposition temperature at 5% weight loss.

Table S2. Sur	nmarized de	evice data	for DBICz-	DPA devices
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Device	Conc. (%)	L _{max} (cd/m ²) ^a	CE _{Max/10000/60000} (cd/A) ^b	EQE _{Max/10000/} 60000 (%) ^c	CIE(x, y) ^d	EL _{max} (nm)	FWHM (nm)
A	3	87480	9.37/9.24/9.00	6.09/6.00/ 5.87	(0.13, 0.23)	472	52
В	5	87991	10.17/10.08/ 9.59	6.22/6.15/ 5.95	(0.13, 0.25)	473	50
С	7	82967	9.64/9.62/8.45	5.90/5.85/ 5.27	(0.13, 0.26)	475	49

^aMaximum luminance. ^bCurrent efficiency at maximum brightness and 10000, 60000 cd/m² brightness. ^cExternal quantum efficiencies at maximum brightness and 10000, 60000 cd/m² brightness. ^dCIE coordinates at about 10000 cd/m² brightness.

Compounds	EQE	L _{max} (cd/m ²)	(x,y)	FWHM (nm)	Lifetime (h)	Ref.
	max 6.22% @10,000 cd/m ² - 6.15% @60,000 cd/m ² - 5.59%	87,991	(0.13,0.2 5)	50	LT ₉₀ >32.9 (@1000 cd/m ²)	This work
	max 7.11% @1000 cd/m ² - 6.59%	-	(0.15, 0.13)	-	LT ₅₀ -55 (@500 cd/m ²)	[5]
× C V	max 9.25%	-	(0.133, 0.145)	37	LT ₉₇ -275 LT ₉₅ -471 (@1000 cd/m ²)	[6]
	max 7.23%	11,970	(0.157. 0.073)	-	LT ₉₀ ~50 h (@100 cd/m ²)	[7]
	max 10.48% @1000 cd/m ² - 7.54%	16,776	(0.15, 0.13)	63	-	[8]
	max 10.27% @1000 cd/m ² - 7.25%	-	(0.15, 0.05)	51	-	[9]
	max 6.01%	370	(0.153, 0.051)	60	-	[10]
	max 4.46% @1000 cd/m ² - 4.42%	20,129	(0.16, 0.23)	-	-	[11]
	max 10.5% @1000 cd/m ² - 4.6%	10,480	(0.152, 0.065)	-	-	[12]

 Table S3 Comparison of current work with the performances of recently reported blue emitters

	max 6.63%	17,007	-	-	-	[13]
	max 4.53% @1000 cd/m ² - 4.34%	12,491	(0.149, 0.105)	-	-	[14]
	max 8.5% @1000 cd/m ² - 4.8%	-	(0.139, 0.189)	58	-	[15]
	max 8.5% @1000 cd/m ² - 4.6%	-	(0.142, 0.116)	56	-	
	max 8.84% @1000 cd/m ² - 7.70%	17,560	(0.15, 0.07)	-	-	[16]
$+ G^{N} G^{N} G^{N} G^{N} G^{N} G^{N}$	max 14.1%	5500	(0.22, 0.19)	-	-	[17]
	max 12.6% @1000 cd/m ² - 9.5%	>6000	(0.15, 0.10)	-	-	[18]
	max 9.23% @1000 cd/m ² - 7.10%	8044	(0.14, 0.10)	63	-	[10]
	max 10.06% @1000 cd/m ² - 8.97%	15380	(0.14, 0.14)	64	-	[13]

$ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	max 6.94% @1000 cd/m ² - 4.97%	~4000	(0.15, 0.09)	-	-	[20]
H,CO	max 8.0% @1000 cd/m ² - 3.9%	6527	(0.15, 0.09)	-	-	[21]
	max 5.2% @1000 cd/m ² - 4.3%	7340	(0.145, 0.093)	-	-	
	max 5.1% @1000 cd/m ² - 3.2%	7800	(0.148, 0.084)	-	-	[22]
	max 5.78%	~7000	(0.153, 0.099)	-	-	[23]



Fig. S7 ¹H-NMR spectrum of DBICz.



Fig. S8 ¹³C-NMR spectrum of DBICz.



Fig. S9 ¹H-NMR spectrum of DBICz-DPA.

148,54 147,32 14



Fig. S10 ¹³C-NMR spectrum of DBICz-DPA.

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