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Multi-triphenylamine-substituted carbazoles: synthesis, characterization, properties, and applications as hole-transporting materials

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ABSTRACT

A series of triphenylamine-substituted carbazoles, namely **TnC** (n = 2-4), are synthesized and characterized. By increasing the number of triphenylamine substituents, we are able to reduce the crystallization and improve the thermal stability of the molecule. Their thermal properties and abilities as hole-transporting layers in Alq3-based OLED, especially **T4C** having four triphenylamine substituents, are greater than both the common hole-transporters, N,N'-diphenyl-N,N'-bis(1-naphthyl)-(1,1'-biphenyl)-4,4'-diamine (NPB) and N,N'-bis(3-methylphenyl)-N,N'-bis(phenyl)benzidine (TPD). A green light-emitting device with a luminance efficiency as high as 5.07 cd/A is achieved.

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Since the pioneering work on the first organic light-emitting diodes (OLEDs) by Tang in 1987,¹ OLEDs have attracted significant attention from the scientific community due to their potential for future flat-panel displays and lighting applications.² The past decade has seen great progress in both device fabrication techniques and material development.^{3,4} One of the key developments is the use of hole-transporting layers (HTLs) for hole injection from the anode into the light-emitting layer providing significant improvements in the performance of devices.⁵ As a result, many new hole-transporting materials (HTMs) have been developed.⁶⁻⁸ In particular, low-molecular weight amorphous materials have received interest as HTM candidates due to their easy purification by vapor deposition or column chromatographic techniques, and uniformly thin films can be processed simply by coating techniques. The most commonly used amorphous hole-transporting materials (AHTMs) are triarylamine derivatives such as N,N'-diphenyl-N,N'-bis(1-naphthyl)-(1,1'-biphenyl)-4,4'-diamine (NPB) and *N*,*N*'-bis(3-methylphenyl)-*N*,*N*'-bis(phenyl)benzidine (TPD), which demonstrate excellent hole-transporting properties. However, their low thermal and morphological stability usually leads to their degradation.⁹ In order to achieve highly efficient and long lifetime devices, an AHTM with high mobility, a high glass transition temperature (T_{σ}) , a stable amorphous state, and good thin film forming ability are desirable. To optimize all these requirements, many efforts have been devoted to the synthesis of new AHTMs.^{6,10} Carbazole derivatives containing a peripheral diarylamine,¹¹ additional carbazole,¹² bis(4-tert-butylphenyl)carbazole,¹³ and dipyrenyl units¹⁴ were also reported to exhibit good thermal and morphological stability. Recently, we synthesized a series of aromatic comperipheral triphenylamine-carbazole pounds with units possessing high T_{g} (121–185 °C) values, and found that the OLED devices based on the resulting carbazole compounds were promising in terms of device performance and stability.¹⁵ Undoubtedly, it is very attractive to explore and develop new carbazole derivatives that meet the requirements as AHTMs for OLEDs, and which can be synthesized using simple and low-cost methods. Our design involved multiple substitution of the carbazole ring with triphenylamine moieties. With this molecular architecture, compounds should exhibit amorphous hole-transporting ability.

Herein, we report on a simple synthesis of multi-triphenylamine substituted carbazoles (**TnC**, n = 2-4), and their physical and photophysical properties. Investigations on their abilities to act as hole-transporting layers in OLEDs are also reported. Scheme 1 outlines the synthesis of the triphenylamine functionalized carbazoles. We began with the synthesis of 3,6-dibromo-*N*-dodecylcarbazole (**2**),





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Scheme 1. Synthesis of triphenylamine substituted carbazoles TnC.

1,3,6-tribromo-N-dodecylcarbazole (3), and 1,3,6,8-tetrabromo-Ndodecylcarbazole (4) by bromination of N-dodecylcarbazole (1) with NBS.¹⁶ A solution of 2 in THF was treated with NBS (2.1-15.0 equiv) in small portions in the absence of light to yield bromides 2-4 in moderate to good yields (75-94%). Subsequently, coupling of these multibromo-N-dodecylcarbazoles 2-4 with 4-(diphenylamino)phenylboronic acid (2.2-5.5 equiv) in the presence of Pd(PPh₃)₄ as the catalyst and aqueous Na₂CO₃ as the base in THF at reflux afforded 3,6-bis[4-(diphenylamino)phenyl]-Ndodecylcarbazole (T2C), 1,3,6-tri[4-(diphenylamino)phenyl]-Ndodecylcarbazole (T3C), and 1,3,6,8-tetrakis(4-(diphenylamino) phenyl)-N-dodecylcarbazole (T4C) as white solids in good yields (75-92%). The structures of the products were characterized unambiguously by ¹H NMR and ¹³C NMR spectroscopy as well as high-res-olution mass spectrometry. ¹⁷ Noticeably, the ¹H NMR spectra of **TnC** showed that the chemical shifts of the dodecyl protons were shifted to low frequency as the number of triphenylamine substituents on the carbazole increased. This is due to a shielding effect resulting from the ring current produced by the surrounding 1- and 8-triphenylamine substituents. For example, the chemical shift of -NCH₂protons of T2C (4.34 ppm) was shifted to 4.00 and 3.70 ppm in T3C and T4C, respectively. These compounds showed good solubility in most organic solvents.

To gain insight into the geometrical and electronic properties of these multisubstituted carbazoles, quantum chemistry calculations were performed using the TDDFT/B3LYP/6-31G(d) method.¹⁸ The optimized structures of the **TnCs** revealed that the phenyl rings attached to the carbazole of each triphenylamine were twisted out of the plane of the carbazole, forming bulky substituents around the carbazole, especially in **T4C** (Fig. 1). This would facilitate the formation of amorphous materials. In all cases, π -electrons in the HOMO orbitals were delocalized only over the carbazole and two triphenylamine substituents at the 3- and 6-positions {3,6-bis[4-(diphenylamino)phenyl]carbazole backbone}, and no electrons at the triphenylamine moieties at the 1 and



Figure 1. HOMO and LUMO orbitals of T2C and T4C calculated by the TDDFT/ B3LYP/6-31G(d) method.

8-positions. In the LUMO orbitals, the excited electrons were delocalized over the carbazole plane and the phenyl ring of the triphenylamine substituents at the 1,8-positions. This suggests that substitution of the carbazole at the 1- or 8-positions with triphenylamine only affected the LUMO of the molecule, while the HOMO remained nearly untouched.

The solution UV–vis absorption spectra of **TnC** showed absorption bands at 320–328 nm corresponding to the π – π * electronic transition of the π -conjugated 3,6-bis[4-(diphenylamino)phenyl] carbazole backbone (Fig. 2a). With **T3C** and **T4C**, absorption bands at lower wavelengths (284–296 nm) were observed, which were identical to the absorption peak of a triphenylamine



Figure 2. (a) UV-vis absorption and PL spectra in CH_2Cl_2 solution (thick line) and thin films (thin line). (b) CV curves measured in CH_2Cl_2 at a scan rate of 50 mV/s. (c) DSC and TGA curves measured with a heating rate of 10 °C/min under N₂. (d) EL spectra of the OLEDs.

chromophore.¹⁹ This absorption band can be assigned to the π - π^* electron transition of the isolated triphenylamine substituents at the 1- or 8-positions. The intensity of this peak was stronger in **T4C** as it has two triphenylamine moieties (1,8-positions). This outcome agrees with the quantum chemistry calculation results. The solution photoluminescence (PL) spectra of **TnC** displayed an emission band in the blue-purple region ($\lambda_{max} = 415-419$ nm). The PL spectra of their thin films were similar to those in solution with a ~10 nm red shift. This indicates the presence of certain intermolecular electronic interactions. Nevertheless, the degree of the red shift is considerably smaller than those observed with π -conjugated compounds that adopt face-to-face stacking.²⁰ These materials show slight Stoke shifts (91–95 nm) suggesting reduced energy loss during the relaxation process.

The CV curves of the **TnC**s measured in CH_2Cl_2 containing *n*-Bu₄NF₆ as the supporting electrolyte exhibited multiple quasireversible oxidation processes (Fig. 2b, Table 1). Under these experimental conditions, no reduction was observed in all cases. The first two oxidation waves at 0.78 and 0.89 V in all the compounds appeared at the same potential and could be assigned to the removal of electrons from the conjugated 3,6-bis[4-(diphenylamino)phenyl]carbazole backbone resulting in a radical cation and dication, respectively. The oxidation waves at 1.03–1.07 V in both **T3C** and **T4C** matched with the oxidation potential of a triphenylamine ($E_{ox} = 0.98$ V vs SCE), and therefore can be assigned to oxidation of the isolated triphenylamine substituent at the 1,8-positions, consistent with both the optical and the quantum chemistry calculation results. The oxidation waves at higher potential

Table 1	
Physical data of the TnCs and their OLED device charac	teristics

Compd	Abs ^a (nm)	Em ^a (nm)	$T_{\rm g}/T_{\rm m}/T_{\rm 5d}{}^{\rm b}$ (°C)	$E_{1/2}^{\text{ox}}$ versus Ag/Ag ^{+c} (V)	Eg (eV) ^d	HOMO/LUMO ^d (eV)	$\frac{V_{\rm on}/V_{100}}{\rm (V)^e}$	λ_{em} (nm)	L _{max} (cd/ m ²)	η (cd/ A)	EQE (%) ^f
T2C T3C T4C NPB TPD	320 296, 325 284, 328 339 352	415 417 419 450 398	-/189/334 78/207/372 122/-/415 100/-/- 63/-/-	0.78, 0.89, 1.20 0.78, 0.89, 1.07, 1.25 0.78, 0.89, 1.03, 1.29 –	3.29 3.26 3.24 	-5.15/-1.86 -5.16/-1.90 -5.15/-1.91 -5.50/-2.40 -5.50/-2.30	2.4/3.0 2.4/3.4 2.5/3.4 2.5/3.6 2.5/3.7	518 518 518 519 518	28781 25052 22411 31857 22539	4.97 5.00 5.07 4.45 4.05	0.24 0.24 0.25 0.22 0.20

^a Measured in CH₂Cl₂ solution. ^b Measured by DSC and TGA.

^c Measured by CV using a glassy carbon working electrode, a Pt counter electrode, and an Ag/Ag⁺ reference electrode with 0.1 M *n*-Bu₄NPF₆ as the supporting electrolyte in CH₂Cl₂.

^d Calculated from: $E_g = 1240/\lambda_{onset}$; HOMO = $-(4.44 + E_{onset}^{ox})$; LUMO = E_g + HOMO.

^e Voltage at a luminance of 1 and 100 cd/m².

^f External quantum efficiency.



Figure 3. (a) *I*–*V*–*L* and (b) η –*I* characteristics of the fabricated OLEDs.

(1.20-1.29 V) of all cases correspond to the removal of electrons from the interior of the carbazole moiety. Multiple CV scans (7 scans) revealed identical CV curves with no additional peak at lower potentials on the cathodic scan (E_{pc}) being observed. This suggests no electrochemical coupling at either the carbazole or triphenylamine peripheries, indicating electrochemically stable molecules. Usually, this type of electrochemical coupling reaction is detected in most triphenylamine derivatives with unsubstituted p-positions on the phenyl ring, such as in the case of 7-(pyren-1yl)-2,9,9-tris(4-diphenylaminophenyl)fluorene.²¹ The steric hindrance effect and stability from electron delocalization might play an important role in protecting the triphenylamine moieties particularly in such electrochemical reactions in all compounds. The HOMO and LUMO energy levels of the TnCs were calculated from the oxidation onset potentials (E_{onset}) and energy gaps (E_g) , and the results are summarized in Table 1. All the compounds had identical HOMO levels of -5.15 V, while their LUMO levels are varied from -1.86 to -1.91 V.

The thermal properties of the TnCs were determined by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) and the results are shown in Figure 2c and Table 1. T2C is a crystalline material as its DSC trace reveals only an endothermic peak due to the melting point at 189 °C, while the thermogram of T4C showed only an endothermic baseline shift due to glass transitions (T_g) at 122 °C, indicating an amorphous material. When the crystalline sample of **T3C** was subjected to a DSC heating scan, an endothermic baseline shift at 78 °C followed by an exothermic peak due to crystallization and an endothermic melting peak at 163 and 207 °C, respectively, were observed, indicating a semicrystalline material. The T_g value of amorphous T4C was higher than those of the most widely used HTMs, NPB ($T_{\rm g}$ = 100 °C), and TPD ($T_g = 63 \text{ °C}$).²² The thermal stabilities of **TnC** were further confirmed by TGA measurements showing an increasing 5% weight loss temperature (T_{5d}) from 334 °C for **T2C** to 415 °C for **T4C** as the number the triphenylamines in the molecule increased. These results suggest that the presence of multiple triphenylamines in the molecule not only improves its thermal stability, but also induces the formation of an amorphous form, which in turn could increase the service time in device operation and enhance the morphological stability of the thin film. Moreover, the ability to form a molecular glass with the possibility to prepare good thin films by both evaporation and solution casting processes is highly desirable for applications in electroluminescent devices.

According to the above discussed excellent properties, the ability of these **TnCs** as a hole-transporting layer (HTL) in OLEDs was investigated. Alq3-based green OLEDs with the following structure of ITO/PEDOT:PSS/**TnC** (spin-coating)/Alq3 (50 nm)/LiF (0.5 nm):Al (200 nm) were fabricated, where Alq3 is the green light-emitting

and electron transporting layer (EML). Under the applied voltage, all the devices exhibited a bright green emission with peaks centered at 517-518 nm and the Commission Internationale de l'Éclairage (CIE) coordinates of (0.29, 0.53) (Fig. 2d). The electroluminescence (EL) spectra of these diodes were identical, and matched with the PL spectrum of Alg3, the EL of the reference devices (NPB and TPD as HTL), and also other reported EL spectra of Alq3-based devices.²³ No emission at a longer wavelength owing to exciplex species formed at the interface of **TnC** and Alg3, which often occurs in the devices fabricated with planar molecules, was detected.²⁴ From these results, and in view of the fact that the barrier for electron migration at the Alq3/TnC interface (~2.10 eV) was significantly higher than those for hole-migration at the **TnC**/ Alq3 interface (~0.36 eV), hence, under the present device configuration, **TnCs** would act only as HTL, and Alq3 would act preferably as an electron blocker more than as a hole blocker with charge recombination thus confined to Alq3 layer. A stable emission was observed in all diodes with the EL spectra and CIE coordinates remaining unchanged over a range of operating voltages. The TnC-based devices exhibited turn-on voltages in the range of 2.4–2.5 V and operating voltages at 100 cd/m² in the range of 3.0-3.4 V, indicating good device performance (Fig. 3 and Table 1). The device with T4C as the HTL displayed the best performance with a high maximum brightness (L_{max}) of 22411 cd/m² at 8.4 V, a low turn-on voltage (Von) of 2.5 V and a maximum luminous efficiency (η) of 5.07 cd/A. A comparable device performance was observed from the **T3C**-based device showing L_{max} of 25052 cd/m² at 8.0 V, $V_{\rm on}$ of 2.4 V and a maximum η of 5.00 cd/A, while the **T2C**based device showed slightly lower device performance. In comparison with the NPB- and TPD-based devices (Table 1), the use of **TnCs** as HTLs clearly improves the device performance, indicating the ability of the **TnC**s as HTMs was superior than NPB and TPD.

In summary, we have demonstrated the simple design strategy, synthesis, and characterization of multi-triphenylamine-substituted carbazoles. Increasing the number of triphenylmine substituents in the molecule not only improved the thermal stability, but also induced the formation of an amorphous form in the material. They are electrochemically and thermally stable materials with reasonably high glass transition temperatures. These materials show excellent hole-transporting properties for Alq3-based green OLEDs with device luminance efficiencies as high as 5.07 cd/A being achieved.

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- Characterization data for **T2C**: mp 170–172 °C; ¹H NMR (300 MHz, CDCl₃): δ 0.90 (3H, t, *J* = 6.9 Hz), 1.27–1.49 (18H, m), 1.93 (2H, t, *J* = 6.9 Hz), 4.34 (2H, t, *J* = 6.6 Hz), 7.05 (4H, t, *J* = 7.5 Hz), 7.20 (12H, t, *J* = 9.3 Hz), 7.30 (8H, t, *J* = 8.4 Hz), 7.46 (2H, d, *J* = 8.4 Hz), 7.63 (4H, d, *J* = 8.7 Hz), 7.72 (2H, d, *J* = 12.0 Hz), 8.35 (2H, s); ¹³C NMR (75 MHz, CDCl₃): δ 14.12, 22.69, 27.34, 29.08, 29.33, 29.43, 29.52, 29.61, 31.91, 43.36, 109.03, 118.45, 122.67, 123.50, 124.18, 124.50, 124.96, 127.88, 129.24, 131.90, 136.47, 140.20, 146.39, 147.87; HRMS calcd for C₆₀H₅₉N₃, *m/z* 821.4709; found; 822.5430 [MH⁺]. Characterization data for **T3C**: mp 120–122 °C; ¹H NMR (300 MHz, CDCl₃): δ

0.87 (3H, m), 1.04–1.23 (20H, m), 4.00 (2H, s), 7.06 (7H, t, J = 9.9 Hz), 7.18–7.33 (29H, m), 7.42 (3H, d, J = 8.4 Hz), 7.54 (1H, s), 7.61–7.72 (5H, m), 8.35 (2H, d, J = 6.3 Hz); ¹³C NMR (75 MHz, CDCl₃): δ 14.16, 22.70, 26.89, 29.34, 29.62, 29.68, 31.92, 109.54, 117.16, 118.20, 122.68, 123.05, 124.14, 124.19, 124.47, 124.53, 125.09, 126.11, 127.91, 129.24, 129.36, 130.66, 146.46, 147.28, 147.77; HRMS calcd for C₇₈H₇₂N₄ m/z 1064.5757; found, 1065.7021 [MH⁺].

Characterization data for **T4C**: mp 128–130 °C; ¹H NMR (300 MHz, CDCl₃): δ 0.53 (3H, t, *J* = 6.9 Hz), 0.83–1.26 (20H, m), 3.70 (2H, s), 7.00–7.08 (9H, m), 7.16 (21H, t, *J* = 4.5 Hz), 7.25–7.32 (18H, m), 7.43 (4H, d, *J* = 8.4 Hz), 7.54(2H, d, *J* = 1.5 Hz), 7.65 (4H, d, *J* = 8.4 Hz), 8.34 (2H, s); ¹³C NMR (75 MHz, CDCl₃): δ 14.13, 22.66, 26.23, 28.63, 29.01, 29.34, 29.50, 29.60, 29.71, 31.88, 45.57, 116.89, 122.69, 122.99, 123.33, 124.16, 124.42, 124.53, 126.07, 126.55, 126.88, 127.91, 128.24, 129.23, 129.33, 130.28, 130.98, 132.37, 134.64, 136.01, 139.04, 146.51, 147.10, 147.76; HRMS calcd for C₉₆H₈₅N₅ *m/z* 1308.6839; found, 1308.9110 [M*].

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