



Carbazole modified terphenyl based high triplet energy host materials for blue phosphorescent organic light-emitting diodes



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ABSTRACT

Carbazole modified terphenyl based high triplet energy host materials were developed for application as host materials for blue phosphorescent organic light-emitting diodes. Two terphenyl based materials, 9-(5''-phenyl-[1,1':2',1'':3'',1'''-quaterphenyl]-3-yl)-9H-carbazole (CzTPPh) and 9-(3'',5''-di(pyridin-3-yl)-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole (CzTPPy), were synthesized as the host materials with high triplet energies of 2.75 eV and 2.73 eV, respectively. The two host materials were evaluated as the host materials for blue phosphorescent organic light-emitting diodes and high quantum efficiencies of 20.2% and 15.7% were obtained in the CzTPPh and CzTPPy devices, respectively.

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1. Introduction

The development of high triplet energy host materials is important to improve the external quantum efficiency of blue phosphorescent organic light-emitting diodes (PHOLEDs) because the efficiency of the blue PHOLEDs mainly depends on energy transfer from host to blue triplet emitter. The triplet energy of the host material should be higher than that of dopant material for efficient energy transfer from host to dopant.

The high triplet energy host materials should be designed to include high triplet energy moieties in the molecular structure [1–20]. Common high triplet energy host materials have carbazole [1–10], fluorene [11–13] and dibenzofuran [14–17] as the high triplet energy moieties in the backbone structure, which was combined with other aromatic units to produce the high triplet energy host materials. In general, aromatic units derived from phenyl or biphenyl backbone structure were used to realize high triplet energy because a terphenyl unit reduced the triplet energy of the host materials. However, the terphenyl unit can be used to develop high triplet energy host materials by decreasing the degree of conjugation through a kink structure [18]. The merits of using the kinked terphenyl core were high triplet energy and high thermal stability.

A few high triplet energy host materials possessing the kinked terphenyl core structure were reported as the host materials for blue PHOLEDs [19–23].

In this work, high triplet energy host materials derived from the carbazole modified kinked terphenyl core structure, 9-(5''-phenyl-[1,1':2',1'':3'',1'''-quaterphenyl]-3-yl)-9H-carbazole (CzTPPh) and 9-(3'',5''-di(pyridin-3-yl)-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole (CzTPPy), were synthesized as the host materials for blue PHOLEDs. A high triplet energy over 2.70 eV was obtained using the CzTPPh and CzTPPy host materials and a high quantum efficiency of 20.2% was achieved using the CzTPPh host material.

2. Experimental section

2.1. General information

All chemicals and reagents were purchased from Aldrich and TCI Chem, and were used without further purification. 3-(9H-carbazol-9-yl)phenylboronic acid was prepared according to the synthetic method in literature [24] and general chemical analysis were described in our previous work [25].

2.1.1. Synthesis of 9-(2'-bromo-[1,1'-biphenyl]-3-yl)-9H-carbazole

3-(9H-carbazol-9-yl)phenylboronic acid (12.0 g, 42.1 mmol), 1,2-dibromobenzene (50.0 g, 211 mmol) and tetrahydrofuran (480 ml) were added to a two-necked flask equipped with a magnetic

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stirring bar, a septum and a reflux condenser attached to a gas-flow adapter with a stopcock. The solution was bubbled with high purity nitrogen gas for 30 min to remove oxygen and potassium carbonate (11.6 g, 84.3 mmol) dissolved in oxygen free distilled water (160 ml) was added to the solution. Tetrakis(triphenylphosphine)palladium(0) ($\text{Pd}(\text{PPh}_3)_4$, 2.43 g, 2.11 mmol) was added and the resulting suspension was refluxed for 24 h under nitrogen. The solution was allowed to cool and was transferred to a separatory funnel. The solution was extracted with ethyl acetate and the organic layer was combined, washed with water saturated with sodium chloride, and dried over magnesium sulfate. Solvent was removed with a rotary evaporator to yield a yellow oil, which was purified by column chromatography (dichloromethane/*n*-hexane) to give 14.0 g of 9-(2'-bromo-[1,1'-biphenyl]-3-yl)-9H-carbazole.

Yield: 84%. ^1H NMR (500 MHz, CDCl_3): δ 7.23 (t, 1H, $J = 6.0$ Hz), 7.29 (t, 2H, $J = 4.8$ Hz), 7.37–7.44 (m, 4H), 7.49 (d, 1H, $J = 4.0$ Hz), 7.52 (d, 2H, $J = 4.0$ Hz), 7.60 (d, 1H, $J = 4.0$ Hz), 7.63 (s, 1H), 7.66 (t, 1H, $J = 5.2$ Hz), 7.70 (d, 1H, $J = 4.0$ Hz), 8.15 (d, 2H, $J = 4.0$ Hz), Mass (FAB): m/z 397 $[\text{M}^+]$.

2.1.2. Synthesis of 9-(3'',5''-dichloro-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole

9-(2'-Bromo-[1,1'-biphenyl]-3-yl)-9H-carbazole (10.0 g, 25.1 mmol), 3,5-dichlorophenylboronic acid (6.23 g, 32.6 mmol) and tetrahydrofuran (240 ml) were added to a two-necked flask and was bubbled with nitrogen for 30 min. Potassium carbonate (8.68 g, 62.8 mmol) dissolved in oxygen free distilled water (80 ml) was added to the solution followed by adding $\text{Pd}(\text{PPh}_3)_4$ (1.45 g, 1.26 mmol). The resulting suspension was refluxed for 24 h under nitrogen. The reaction was allowed to cool and was extracted with ethyl acetate. The organic layer was combined, washed with water saturated with sodium chloride, and dried over magnesium sulfate. Solvent was removed with a rotary evaporator to yield a brown powder, which was purified by column chromatography using a dichloromethane/*n*-hexane eluent to give 9-(3'',5''-dichloro-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole (9.0 g) as a white powder.

Yield: 77%. ^1H NMR (500 MHz, CDCl_3): δ 7.01 (d, 2H, $J = 4.0$ Hz), 7.13 (s, 2H), 7.23 (s, 1H), 7.26 (t, 1H, $J = 4.8$ Hz), 7.33–7.51 (m, 10H), 7.59 (t, 1H, $J = 5.2$ Hz), 8.10 (d, 2H, $J = 4.0$ Hz). Mass (FAB): m/z 463 $[\text{M}^+]$.

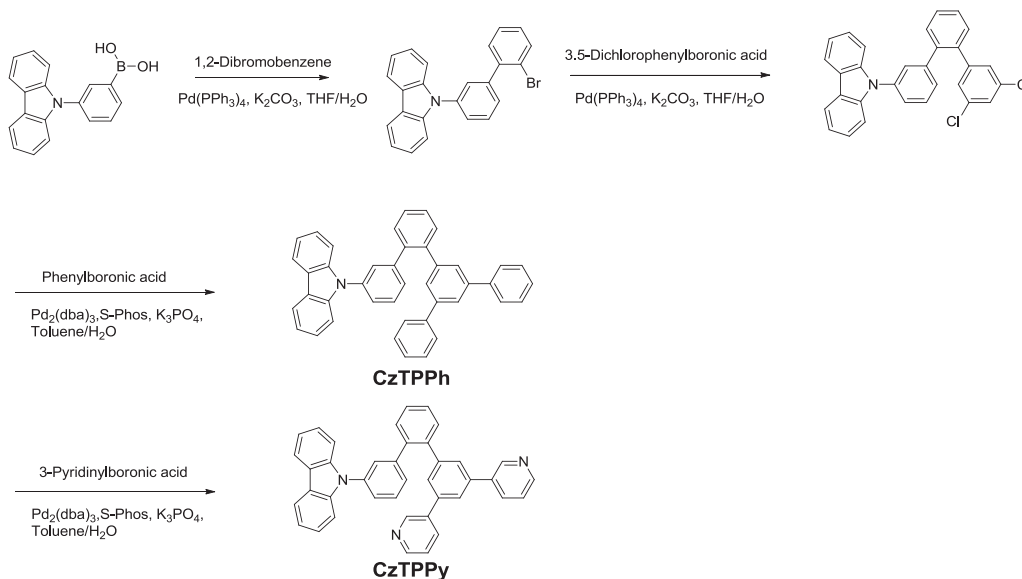
2.1.3. 9-(5''-Phenyl-[1,1':2',1'''-quaterphenyl]-3-yl)-9H-carbazole (CzTPPh)

A solution of 9-(3'',5''-dichloro-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole (3.00 g, 6.46 mmol), phenylboronic acid (3.15 g, 25.8 mmol), K_3PO_4 (8.23 g, 38.8 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (S-Phos, 0.53 g, 1.29 mmol), tris(dibenzylideneacetone)dipalladium ($\text{Pd}_2(\text{dab})_3$, 0.30 g, 0.34 mmol), toluene (210 ml) and distilled water (21 ml) was refluxed for 48 h. The solution was cooled down to room temperature, diluted with 100 ml water and extracted with ethyl acetate. The organic extracts were dried over anhydrous magnesium sulfate, filtered, and evaporated to yield a brown solid. The crude product was purified by column chromatography on silica gel using dichloromethane/*n*-hexane as an eluent. Additional purification by sublimation (250 °C. at 10^{-5} mmHg) resulted in 1.5 g of pure glassy solid.

Yield: 42%. T_g : 90 °C, T_m : 176 °C. FT-IR (ATR): 3053, 1592, 1476, 1450, 1412, 1312, 1228, 1164, 1081, 1028, 880, 802, 749, 697 cm^{-1} . ^1H NMR (500 MHz, CDCl_3): δ 7.03 (d, 2H, $J = 4.3$ Hz), 7.18 (t, 4H, $J = 8.3$ Hz), 7.32 (t, 2H, $J = 4.8$ Hz), 7.39 (t, 4H, $J = 5.0$ Hz), 7.42–7.50 (m, 11H), 7.54–7.61 (m, 3H), 7.78 (s, 1H), 8.04 (d, 2H, $J = 4.3$ Hz). ^{13}C NMR (125 MHz, CDCl_3): δ 109.6, 119.8, 120.1, 123.3, 124.4, 125.0, 125.9, 127.3, 127.5, 127.8, 128.0, 128.1, 128.6, 128.8, 129.7, 130.6, 137.5, 140.0, 140.3, 140.7, 140.9, 141.9, 142.0, 143.9. Mass (FAB): m/z 547 $[(\text{M})^+]$. Elemental analysis Calcd. for $\text{C}_{42}\text{H}_{29}\text{N}$: C, 92.11%; H, 5.34%; N, 2.56%. Found: C, 92.11%; H, 5.33%; N, 2.58%.

2.1.4. 9-(3''',5''-di(pyridin-3-yl)-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole (CzTPPy)

A solution of 9-(3'',5''-dichloro-[1,1':2',1''-terphenyl]-3-yl)-9H-carbazole (3.00 g, 6.46 mmol), 3-pyridinylboronic acid (3.18 g, 25.8 mmol), K_3PO_4 (8.23 g, 38.8 mmol), S-Phos (0.53 g, 1.29 mmol), $\text{Pd}_2(\text{dab})_3$ (0.30 g, 0.34 mmol), toluene (210 ml) and distilled water (21 ml) was refluxed for 48 h. The solution was cooled down to room temperature, diluted with 100 ml water and extracted with ethyl acetate. The organic extract was dried over anhydrous magnesium sulfate, filtered, and evaporated to yield a brown solid. The crude product was purified by column chromatography on silica gel using dichloromethane/*n*-hexane as an eluent. Additional purification by sublimation (250 °C. at 10^{-5} mmHg) resulted 1.7 g of pure glassy solid.



Scheme 1. Synthetic scheme of CzTPPh and CzTPPy.

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