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Triphenylene containing host materials with high thermal stability for green phosphorescent organic light emitting diode

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A B S T R A C T

We report series of triphenylene derivatives with good electronic properties for the use as host materials for green phosphorescent organic light emitting diodes (PHOLEDs). We applied highly planar triphenylene moieties which could provide good electron transport ability and the carbazole or dibenzothiophene moieties which could provide good hole transport ability to obtain a bipolar host materials for green PHOLEDs. From this approach we achieved relatively good current efficiency up to 64 cd/A and external quantum efficiency up to 20.3%, respectively. This was the much more improved value (by ~22.3%) compare to that obtained from the 4,4′-*N*,*N*′-dicarbazolebiphenyl system as a reference.

1. Introduction

Phosphorescent organic light-emitting diodes (PHOLEDs) have attracted intense interest because of their merit of high quantum efficiency as compared to conventional fluorescent OLEDs through utilizing both singlet and triplet excitons for emission [1–4]. In fact, red phosphorescent materials have already been applied in the main-display of commercial mobile phones since 2007. Recently, green emission is almost approaching to the theoretical limitation of efficiency (>20% of external quantum efficiency, EQE) by utilizing various dopants such as *fac*-tris(2-phenylpyridinato)iridium(III) [Ir(ppy)$_3$] as the phosphorescent emitter, and the commercialization of which has been successfully started [5–9]. However, compared with the great achievements in red phosphorescent materials, green component has many obstacles against commercialization including its relatively short lifetime issue. To overcome such issue, the mixed host system is widely utilized [10–12]. However, many research groups are concentrating on preparation of the host materials which possess bipolar characteristics because the minute change of mixing ratio of hole transport type and electron transport type host materials could change the resultant device characteristics. For this purpose, many achievements have been reported in this field in recent years [2,13,14]. Especially, the host materials with hole transport type functional groups such as carbazoles or triarylamine moieties combined with electron transport type functional groups such as heterocyclic moieties such as pyridine, triazine, benzimidazole showed great progress in the device performances [15,16]. Aryl silanes [17,18] and phosphine oxides [19–21] have also been utilized to obtain bipolar properties as electron transport type functional groups [22]. As a part of such an effort, the efficiency greater than 20% (EQE) was frequently reported from the green PHOLEDs with such kinds of bipolar host materials [23,24].

In this study, we report three different types of new host materials for green PHOLEDs having triplet energy greater than 2.5 eV with highly planar triphenylene moieties to improve their electron transport ability. The resultant PHOLEDs containing such moieties showed moderate EQE up to 20.3%.

2. Results and discussion

2.1. Materials

We prepared three host materials to realize a highly efficient green PHOLED. We selected triphenylene moiety as a basic

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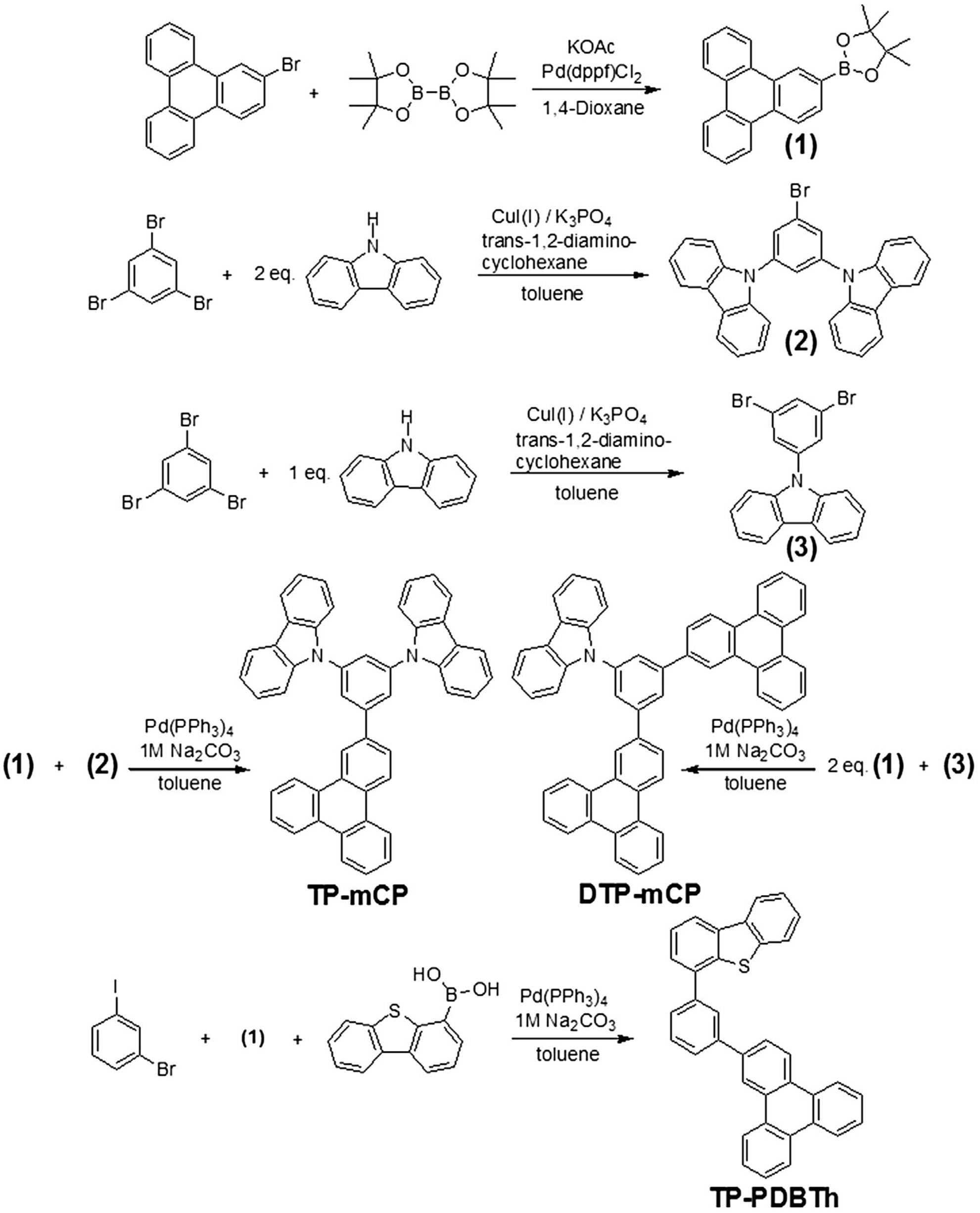
functionality because they are renowned as discotic liquid crystalline molecules for their potential in one-dimensional charge transporting properties. Conductivity along the columns in columnar mesophases has been reported to be several orders of magnitude greater than that in the perpendicular direction. The triphenylene and its derivatives have been known as hole transporting materials although it could also be used as an electron transporting functionality [25] Their photoinduced charge-carrier mobilities ranged from 10^{-5} cm^2 V^{-1} s^{-1} in the isotropic phase [26] to 10^{-2} cm^2 V^{-1} s^{-1} in highly ordered discotic mesophases [27] Meanwhile, we changed the numbers of triphenylene moieties which are connected to the central core unit (1,3,5-trisubstituted benzene) which also contains a hole transporting functional groups such as carbazole and/or dibenzothiophene units. In principle, carbazole containing host materials exhibit high triplet energies if they have no extended π-conjugation length [28,29]. In other words, the most common approach to increase a triplet energy level as a green host might be the disruption of π-conjugation just as in the case of 9,9′-(1,3-Phenylene)bis-9H-carbazole which has two carbazole units connected meta position of a single benzene ring. Scheme 1 shows the schematic diagram of synthetic route to prepare such compounds. Fig. 1 shows the geometries of core parts of those three resultant host materials obtained from the simulation at a DNP/GGA(PBE) level of theory using Dmol3 module (Material Studio 6.1, Accelrys software). The triphenylene moieties were rather twisted to the core benzene unit which could arouse a broken conjugation as we expected and we could utilize those materials as a green host materials ($T_1 > 2.6$ eV). Besides, the molecular orbital distribution of 9,9′-(5-(triphenylen-2-yl)-1,3-phenylene)bis(9H-carbazole) (TP-mCP), 9-(3,5-di(triphenylen-2-yl)phenyl)-9H-carbazole (DTP-mCP), and 4-(3-(triphenylen-2-yl)phenyl)dibenzo[b,d]thiophene (TP-PDBTh) are also shown in Fig. 1. As we expected from the molecular structure, the electrons in highest occupied molecular orbital (HOMO) was localized on the



Scheme 1. Synthesis of green host materials.