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Thermally-stable 2,3-diphenylated benzotiophene containing host materials for red phosphorescent organic light-emitting diodes

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ABSTRACT

This study reports a series of benzo[b]thiophene (BT) derivatives with good electronic properties as host materials for red phosphorescent organic light-emitting diodes (PHOLEDs). We applied thermally-stable materials for red PHOLEDs which contain BT and carbazole moieties which also provide a good charge transport ability, as well as a good charge confinement effect (T_1 > 2.25 eV). To control the appropriate charge transporting ability, two different structures having one or two carbazole units connected to the single BT moiety were prepared. Using this approach, we found that the material with a single carbazole and a single BT unit showed the best current efficiency and external quantum efficiency (up to 23.6 cd/A and 12.8%, respectively). The results of the experiment also suggest that BT could be used as an electron-transporting unit when utilized with carbazole moiety, although it has previously been utilized as a *p*-type material.

1. Introduction

Phosphorescent organic light-emitting diodes (PHOLEDs) have attracted much attention because of their high quantum efficiency as compared to conventional fluorescent OLEDs through utilizing both singlet and triplet excitons for emission [1–5]. In fact, red phosphorescent materials have already been applied in the main-display mode of commercial mobile phones since 2007. Green PHOLEDs have been utilized in the same application as well. More specifically, there has been progress in research on the external quantum efficiency (EQE) of PHOLEDs. Kim and co-authors reported that their extremely high efficiency (>30% of EQE) could be achieved if horizontally-oriented emitters are used [6]. Hence, numerous attempts have been undertaken to combine this extremely high efficiency with high device stability. To make such devices, many ideas are still needed on how to extract the internally trapped emission on a waveguide or a substrate mode. However, the development of thermally or electrochemically stable host materials to improve lifetime and internal quantum efficiency still needs to realize highly stable PHOLEDs, because PHOLEDs generally have a much shorter lifetime compared to fluorescent ones. Indeed, PHOLEDs normally need a more or less complicated evaporation system, such as mixed host approach, to obtain a much longer lifetime, although a very high efficiency could sometimes be achieved from a single host system [7,8]. Thus, many research groups focus on the elaboration of ideal host materials with bipolar characteristics, as a minute change in mixing the ratio of hole transport type and electron transport type host materials could change the resultant device characteristics, as well as negatively impact the reliability of active matrix OLED products. To synthesize the bipolar host material, attempts have been made to combine the hole transport type functional groups, with the electron transport type functional groups, As a result of these efforts, improvements of the PHOLED device efficiency by using certain bipolar host materials have been reported [9–13].

This study reports two different types of new host materials for red PHOLEDs having high triplet (>2.25 eV) with thermally-stable benzo[b]thiophene (BT) moieties to improve their electron transport ability. As a result of using BT moieties at host material, PHOLEDs devices that have novel host materials showed an improved EQE (up to 12.8%).

2. Results and discussion

2.1. Materials

Two bipolar host materials to realize a highly efficient thermally-stable red PHOLEDs were prepared. Due to its frequent

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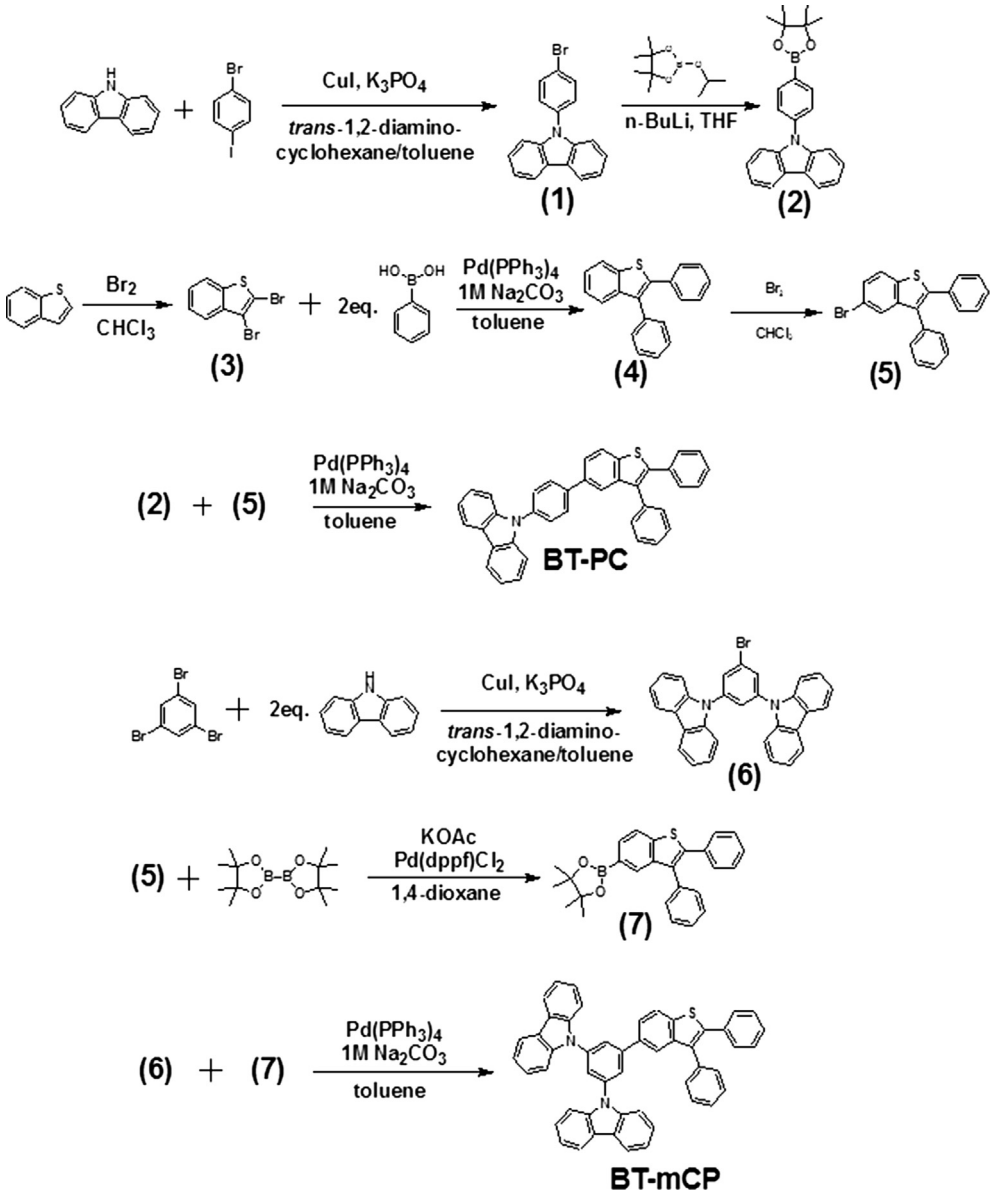
occurrence in nature and useful properties in material science, BT moiety was selected as a basic functionality [14–17]. In particular, the triplet energy level of BT (~2.99 eV) is similar to that of 9-H or 9-phenyl carbazole (~3.01 eV) [18–21]. This is a very useful merit for making new host materials and tuning their triplet energy levels. On the other hand, these BT derivatives including multiply arylated benzo[b]thiophenes and further π-extended benzo[1,2-b;4,5-b′] dithiophenes have recently aroused considerable interest in the field of organic electronics [22–24]. However, to the best of our knowledge, no OLEDs using host materials based on BT moiety have been investigated to date.

Scheme 1 shows the schematic diagram of the synthetic route to prepare such compounds. Herein the 2,3-diphenylated BT derivative was used as an electron-transporting functionality. Indeed, there have scarcely been any attempts to make new bipolar host materials that do not contain any electron-transporting moieties, such as pyridine, triazine, benzimidazole, phosphine oxide, and so on. Meanwhile, we changed the numbers of carbazole moiety connected to the central benzene core unit which act as hole transporting functional units.

Fig. 1 shows the geometries of the core parts of the two resultant host materials obtained from the simulation at a DNP/GGA(PBE) level of theory using Dmol3 module (Material Studio 7.0, Accelrys). BT moieties were rather twisted to the core benzene unit (dihedral angles ca. 38.75–42.05°) which could expectedly arouse a broken conjugation so that these materials can be used as red host materials ($T_1 > 2.25$ eV). In addition, the molecular orbital distribution of *Synthesis of* 9,9′-(5-(triphenylen-2-yl)-1,3-phenylene)bis(9H-carbazole) (BT-mCP), and Synthesis of 9-(4-(2,3-diphenylbenzo[b] thiophen-5-yl)phenyl)-9H-carbazole (BT-PC) are also shown in Fig. 1. As expected from the molecular structures, the electrons in lowest unoccupied molecular orbital (HOMO) were localized on the N-phenylcarbazole (PC) or 1,3-Bis(N-carbazolyl)benzene (mCP) units, while the electrons in lowest unoccupied molecular orbital (LUMO) were dispersed over the 2,3-diphenylbenzo[b]thiophene core units. In other words, the hole carriers injected from the hole



Scheme 1. Synthesis scheme of novel red host materials.