

Balancing charge carrier mobility by constructing chemical structures to contain both hole- and electron-transporting moieties in electroluminescent organic compounds

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Abstract

For the purpose of balancing charge carriers' transport, we designed and synthesized two new compounds that are composed of both electron- and hole-transporting structural moieties: electron-transporting moieties are diaryl-1,3,4-oxadiazole (**Oxa**) groups and hole transport moieties carbazole (**Cz**), or triphenylamine (**TPA**) moieties. The compounds formed amorphous glassy films when vacuum deposited and their glass transition temperature (T_g) was close to or higher than 150 °C. Their electronic structures (the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and E_g values) and hole and electron mobilities in the compounds were studied. A couple of compounds bearing oxadiazole moieties revealed the electron mobility greater than $1.0 \times 10^{-4} \text{ cm}^2/(\text{V s})$ at the electric field of $7.5 \times 10^5 \text{ V/cm}$. The single layer light-emitting electroluminescence (EL) devices show that the external quantum efficiencies of the devices fabricated with those compounds having balanced carrier mobilities are much higher than those of the compounds composed of predominantly hole- or electron-transporting moieties.

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1. Introduction

Electroluminescence (EL) of various organic compounds is attracting much interest since the Eastman Kodak group's first report [1] in 1987 on the EL properties of the devices constructed with a hole-transporting layer and a light-emitting layer. Since then, many electroluminescence devices have been the subject of intensive research in search for better performing systems. Organic light-emitting diodes (OLED) emit light through the following mechanism: initially, negative electrons and positive holes are injected from the electrodes directly into the emitting layer or through transport layers and move toward the opposite electrode. Some of them combine

to form excitons in the emissive layer. These excitons are deactivated to the ground state accompanied by light emission.

In the ideal devices, carrier injection and carrier transport from both electrodes should be balanced. If only one type of charge carriers is injected and transported preferentially, the two opposite charge carriers will not effectively recombine with another one to form excitons. It then would result dominantly in a hole or electron current lowering the device efficiency [2–6].

Among many structural variables to be taken into consideration when one designs the structure of the emitting materials, balanced carrier mobility is one of the most important requirements necessary for high efficiency of light-emitting diodes (LEDs) [2].

In order to achieve the balance in the transport of the two opposite charge carriers, we designed the structure of

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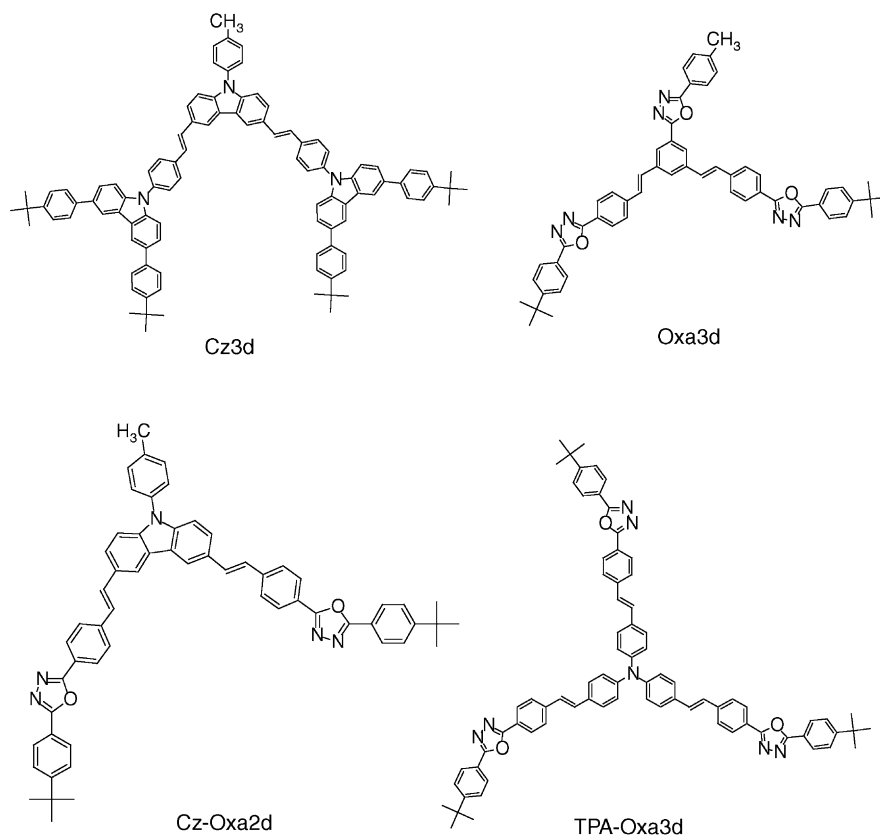


Fig. 1. Structures of compounds.

compounds to have a specific feature that ensures the presence of both electron-transporting diaryl-1,3,4-oxadiazole groups, and the hole-transporting carbazole or triphenylamine moiety centers. The first compound is 3,6-bis-(2-{4-[5-(4-*tert*-butyl-phenyl)-1,3,4-oxadiazol-2-yl]-phenyl}-vinyl)-9-(4-methylphenyl)-9H-carbazole (**Cz-Oxa2d**) and the second tris-[4-(2-{4-[5-(4-*tert*-butyl-phenyl)-1,3,4-oxadiazol-2-yl]-phenyl}-vinyl)-phenyl]amine (**TPA-Oxa3d**) whose chemical structures are shown in Fig. 1. For the sake of comparison, other compounds (**Cz3d** and **Oxa3d**) composed solely of hole- or electron-transporting structures are included in this study. It should be noted from the chemical structures shown in Fig. 1 that carbazole, oxadiazole, and triphenylamine moieties in the compounds are interlinked through the vinylene (–CH=CH–) units. **Cz**, **Oxa**, and **TPA** stand for the carbazole, oxadiazole, and triphenylamine moieties, respectively, and **2d** and **3d** signify the presence of two or three double or vinylene linkers.

In this paper, we describe charge carrier mobility characteristics of the four compounds (**Cz3d**, **Oxa3d**, **Cz-Oxa2d**, and **TPA-Oxa3d**) and luminescence properties of single layer EL devices of **Cz-Oxa2d** and **TPA-Oxa3d** are compared with those of the other two compounds. Information on the electronic structure of the compounds also was studied by UV–vis absorption spectroscopy and cyclovoltametry. The EL properties of **Cz3d** and **Oxa-3d** were reported earlier by us [7].

2. Experimental

2.1. Synthesis

The synthetic route to the preparation of the new compounds, **Cz-Oxa2d** and **TPA-Oxa3d**, are shown in Scheme 1 and the synthetic details can be found elsewhere [8]. Reactions between haloaromatics and styrene derivatives are known to be the Heck reaction [9], which was utilized earlier by us [10] in the synthesis of the structurally related compounds **Cz3d** and **Oxa3d**. Since the synthesis of intermediates was described in detail in our previous reports [7,10], only the details of the last synthetic step are given below.

2.1.1. 3,6-Bis(2-{4-[5-(4-*t*-butyl-phenyl)-1,3,4-oxadiazole-2-yl]phenyl}-vinyl)-9-(4-methylphenyl)-9H-carbazole (**Cz-Oxa2d**)

Compound 4 (1.7 g, 5.6 mmol) and 3,6-dibromo-9-*p*-tolyl-9H-carbazole (0.95 g, 2.3 mmol) were dissolved in 20 mL of *N,N*-dimethyl formamide (DMF) and 10 mL of triethylamine. The mixture was heated slowly and kept at 90 °C under nitrogen atmosphere for 30 min and then added into the reaction mixture were palladium(II) acetate (67 mg, 0.3 mmol) and tri-*o*-tolylphosphine (180 mg, 0.6 mmol). It was stirred for 12 h at 90 °C. After the completion of the reaction, the mixture was cooled down to room temperature.

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