Chinese Chemical Letters Vol. 13, No. 3, pp 256 – 257, 2002
http://www.imm.ac.cn/journal/ccl.html

Novel Blue Light-emitting PPV-based Copolymer Containing Triazole and Carbazole Units

Ze LIU, Li Xiang WANG*, Xia Bin JING, Fo Song WANG

The State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022

Abstract: A novel alternating conjugated copolymer containing triazole and carbazole units was synthesized by the Wittig reaction. The resulting bipolar conjugated polymer emits a pure light with good thermal stability, which is a promising candidate for polymer light emitting display.

Keywords: Light-emitting polymer, photoluminescence, triazole, carbazole.

For making the polymer light-emitting diode (PLED) device with good performance, it is desirable to reach the balance of electron and hole injection. However, for most conjugated polymer, hole injection is more favorable than electron injection. So it is important to design and synthesize the bipolar conjugated polymer with both electron and hole transporting ability for the fabrication of single-layer PLED[1-2].

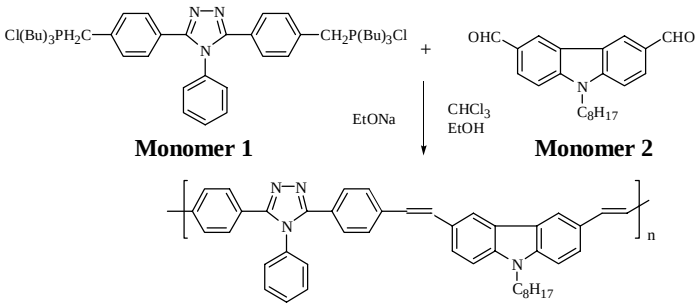
In this communication we present the synthesis and preliminary characterization of new blue light-emitting PPV-based copolymer containing triazole and carbazole moieties (TAZ-CAR-PPV). The design of the copolymer is based on the following facts: 1, 2, 4-triazole and its derivatives have been widely used as electrons transporting materials; the compounds containing carbazole unit are known as hole-transporting materials[3-4].

The synthetic route for TAZ-CAR-PPV is outlined in **Scheme 1**, monomer **1** was obtained from *p*-methylbenzoic acid as starting material through five-step reactions[5]. The monomer **2** was synthesized by the procedure described in literature[4]. TAZ-CAR-PPV was obtained through Wittig condensation polymerization and confirmed by elemental analysis.

TAZ-CAR-PPV is a yellow solid and soluble in organic solvents such as chloroform ($CHCl_3$), tetrahydrofuran (THF). Its average molecular weight (Mw) was measured to be 7944 against the polystyrene standards, with polydispersity around 1.2. TAZ-CAR-PPV shows a decomposition temperature higher than 440°C under nitrogen and a glass transition temperature (T_g) at 147°C, indicating that the introduction of triazole building block into the polymer backbone significantly enhances the thermal stability of the resulting polymer.

* E-mail: lixiang@ns.ciac.jl.cn

Scheme 1 Synthetic route for TAZ-CAR-PPV



UV-Vis absorption and fluorescence spectra data obtained form the solution and films are shown in **Table 1**. Three absorption peaks around 250, 300 and 370 nm are observed, corresponding to the characteristic of the triazole, carbazole units and conjugated backbone. Its PL spectrum appears at 437 nm for the solution and 460 nm for the solid state, indicating that TAZ-CAR-PPV emits pure blue color in film. Compared with similar bipolar conjugated polymer PPOX-CAR containing oxadiazole and carbazole moieties (λ_{PL} = 495 nm), its emission peak is blue-shifted by 35 nm, implying that the triazole unit also plays the rigid spacer role in determining the emission color of the copolymer[4]. Its HOMO, LUMO energy levels and band gap (Eg) are determined by cyclic voltammetry to be –5.26, –2.55 and 2.71 eV, respectively, as listed in **Table 1**.

Table 1 Optical and electronic parameters for TAZ-CAR-PPV

Polymer	λ abs (nm)	PL (sol) (nm)	PL (film) (nm)	Eg[a] (eV)	Eox[b] (V)	Ered[b] (V)	HOMO[b] (eV)	LUMO[b] (eV)	Eg[c] (eV)
TAZ-CAR-PPV	250 300 370	437	460	2.75	0.46	–2.25	–5.26	–2.55	2.71

[a]π-π^* band gap Eg was calculated from the onset of UV absorption (film). [b]Eox and Ered were the value their corresponding redox onset vs ferrocence. [c]π-π^* band gap Eg was calculated from the onset of cyclic voltammetry.

References

1. A. Kraft, A. C. Grimsdale, A. B. Holmes, *Angew. Chem*., *Int. Ed*., **1998**, *37*, 402.
2. J. Kalinowski, *J. Phys. D: Appl. Phys*., **1999**, *32*, 179.
3. P. L. Burn, A. W. Grice, A. Tajbakhsh, D. D .C. Bradley, A. C, Thomas, *Adv. Mater*., **1997**, *9*,1171.
4. S. Y. Song, M. S. Jang, H. K.Shim, D. H. Hwang, T. Zyung, *Macromolecules*., **1999**, *32*, 1482.
5. Z. Liu, L. X. Wang, X. B. Jing, F. S. Wang, *Chem. Mater*., (in press).

Received 28 June, 2001