Synthesis and Characterization of 6,13-Disubstituted Pentacene Derivative

Heung-Gyu Kim[1], E-Joon Choi[1]*, Jae-Hoon Park[2] and Jae-Hoon Kim[2]
[1]Dept. of Polymer Science and Engineering, Kumoh National Institute of Technology, Gumi, 730-701, Korea
TEL: 82-54-478-7684, e-mail: ejchoi@kumoh.ac.kr
[2]Dept. of Electrical and Computer Engineering, Hanyang University, Seoul, 133-701, Korea

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Abstract

Pentacene has excellent semi-conducting characteristics. But pentacene practically used in OTFTs gives rise to problems mainly due to its sensitivity to oxygen and its very low solubility. In order to make up the problems, 6,13-disubstituted pentacene derivative was synthesized and characterized. The properties of the compound were characterized by FT-IR, NMR and we measured the charge transport mobility and the on/off current ratios.

1. Introduction

During the last few years, the development of organic thin film transistors (OTFTs) has attracted much interest.[1-3] The production of OTFTs has been studied because organic molecules offer the opportunity of deposition over large surface areas and are compatible with flexible plastic substrates. Organic materials have the key advantage of potentially simple and low temperature thin film processing by using techniques such as spin coating, stamping or ink-jet printing methods. Thin film field-effect transistors using pentacene as the active semi-conductor have shown a charge transport mobility in the range of 0.005-2.1 $cm^2V^{-1}s^{-1}$ and an on/off current ratios larger than 10^8. But pentacene practically used in OTFTs gives rise to problems mainly due to oxidation and its very low solubility. In this study, we designed, synthesized (see Scheme 1) and characterized new pentacene derivative.

2. Experimental

Measurements. A Jasco 32 FT-IR spectrometer was used to record IR spectra. ^{1}H-NMR spectra was recorded with the used of Bruker 200MHz, and chemical shift were reported in ppm units with tetramethylsilane as internal standard. The electrical properties were obtained at room temperature under dark by ELECS.

Synthesis of 6,13-pentacenequinone (1). 1,4-cyclohexanedione (1.25 g, 11.2 mmol) and potassium hydroxide (2.5 g, 44.8 mmol) were dissolved in ethanol at 0℃. O-phthalaldehyde (3 g, 22.4 mmol) were added to the solution. The reaction mixture was stirred at 0℃ for 1h and at 60℃ for overnight. After the reaction, the product was collected by filteration and then washed with water and ethanol thoroughly.[4]

Synthesis of 6,13-bis(4-propylphenyl)-6,13-dihydro-pentacene 6,13-diol (2). n-BuLi in hexane (2 M, 2 mL, 4 mmol) was added dropwise to a solution of 1-bromo-4-propyl-benzene (0.4 g, 3.9 mmol) in dry THF (20 mL) at -78℃ under nitrogen. The solution was stirred for 40 min. After addition of 6,13-pentacenequinone (0.3 g, 0.975 mmol), the reaction mixture was stirred at -78℃ for 1 h and at room temperature for 7 h. The mixture was poured into water (200 mL) and dichloromethane (100 mL) was added. The organic layer was separated and washed with water (200 mL×2) and then the solvent was removed.

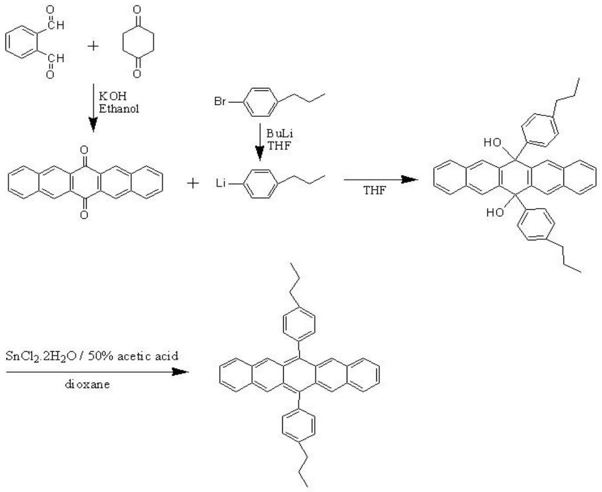
Synthesis of 6,13-bis(4-propylphenyl)pentacene (3). Tin(Ⅱ)chloride dehydrate (2 g, 8.8 mmol) and 50% acetic acid (2 mL) were added to a solution of 6,13-bis(4-propylphenyl)-6,13-dihydropentacene

-6,13-diol (0.5 g, 0.91 mmol) in 1,4-dioxane (80 mL) under nitrogen. The reaction mixture was stirred at 70℃ for 5 h. The mixture was poured into water (200 mL) and dichloromethane (200 mL) was added. The organic layer was separated and washed with water (200 mL×2). After removal of the solvent, the residue was chromatographed on silica gel (hexane/$CHCl_3$ = 1:2) to afford 6,13-bis(4-propylphenyl) pentacene.

Fabrication of organic thin film transistor. The thin film transistors were fabricated with glass substrates. In the first step, a gate electrode was prepared on the glass substrate. Cross-linked polyvinylphenol(CPVP) was used as the insulator. The active layer was made as droping the solution of pentacene derivative (3wt%) in chloroform. The layer was deposited at 260℃ under 10^{-3} Torr for 1 h.

3. Results and discussion

Pentacene derivative was synthesized as shown in Scheme 1. First, 6,13-pentacenequinone reacted with aryllithium to afford the corresponding diarylpentacenediol (see Fig. 1 and Fig. 2). Next, pentacene derivative was prepared by a reaction of the diarylpentacenediol with Tin(Ⅱ) chloride dehydrate in refluxing acetic acid (see Fig. 3 and Fig. 4). The obtained compounds were characterized by FT-IR and NMR. The results were in accordance with exported formula. The synthesized pentacene derivative was soluble to organic solvents such as THF, dichloromethane and chloroform. But it was oxidized in solution under room light at about 20 min. Previously it was reported that other pentacene derivatives could be oxidized under atmosphere with room light.[5] In this study, we could increase the solubility of pentacene although we could not solve the problem of oxidation completely. The electrical properties of pentacene derivative were obtained in TFT with a channel length of 50 μm and a width of 100 μm as shown in Fig. 5. The charge transport mobility was 0.0001 $cm^2V^{-1}s^{-1}$ and an on/off ratio was less than 10^2.



Scheme 1. Synthetic route to 6,13-bis(4-propylphenyl) pentacene.

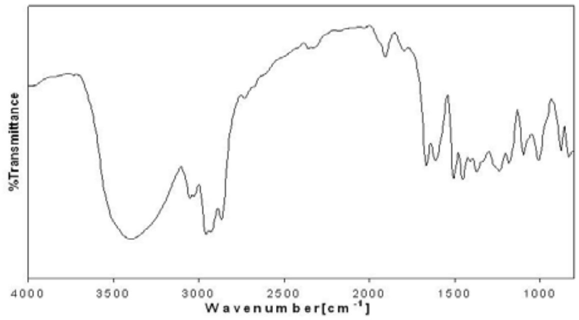


Fig. 1. IR spectrum of 6,13-bis(4-propylphenyl)-6,13-dihydropentacene-6,13-diol (KBr pellet).

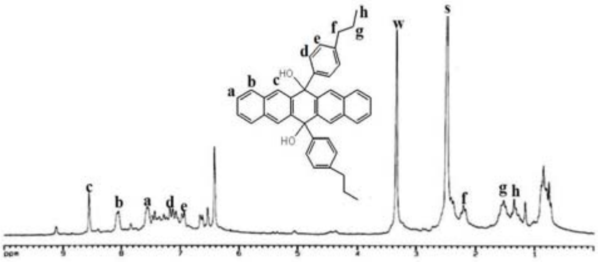


Fig. 2. ^{1}H-NMR spectrum of 6,13-bis(4-propylphenyl)-6,13-dihydropentacene-6,13-diol (solvent = DMSO).

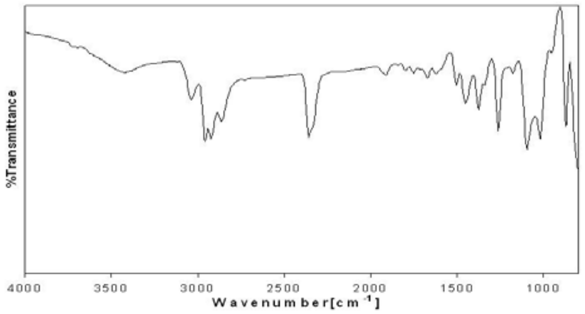


Fig. 3. IR spectrum of 6,13-bis(4-propylphenyl) pentacene (KBr pellet).

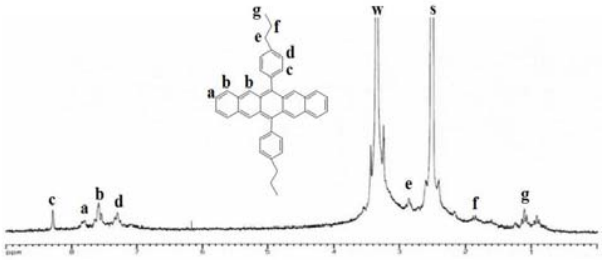


Fig. 4. ^{1}H-NMR spectrum of 6,13-bis(4-propyl phenyl)pentacene (solvent = DMSO).

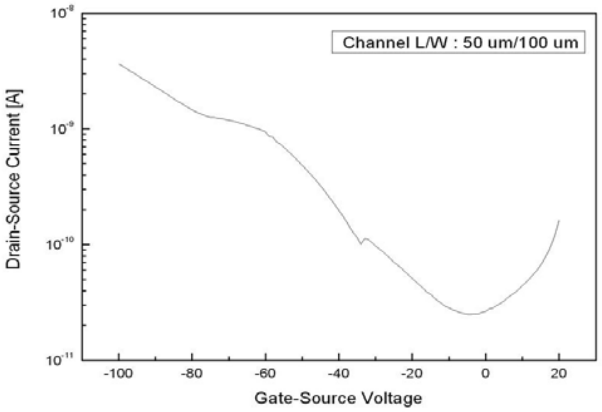


Fig. 5. Transfer characteristic of a pentacene derivative TFT.

4. Summary

New pentacene derivative with flexible side groups has bean synthesized and characterized. 6,13-bis(4-propylphenyl)pentacene is soluble to organic solvents such as chloroform, THF and dichloromethane. Propylphenyl groups of 6,13-bis(4-propylphenyl) pentacene were oxidized in solution under a room light at about 20 min. The charge transport mobility was 0.0001 $cm^2V^{-1}s^{-1}$ and the on/off ratio was less than 10^2. Thereby, we need to improve the structure of the pentacene derivative and the processing.

5. References

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