Organic Electronics 17 (2015) 319–324

Contents lists available at ScienceDirect

Organic Electronics

journal homepage: www.elsevier.com/locate/orgel

Increased photooxidation stability of pentacene derivatives linked with aromatic groups for OTFTs

Dong-Su Kim [a], Ji Eun Jung [a], Nam Seob Baek [b,*], Tae-Dong Kim [a,*]

[a] Department of Advanced Materials, Hannam University, Daejeon 305-701, Republic of Korea
[b] Chem Optics Inc., Daejeon 305-510, Republic of Korea

ARTICLE INFO

Article history:
Received 4 October 2014
Received in revised form 13 November 2014
Accepted 26 November 2014
Available online 24 December 2014

Keywords:
Pentacene derivatives
Photooxidation
Solution-processing
Substituent effects

ABSTRACT

Pentacene derivatives linked with aromatic groups at the 6,13-positions have been synthesized and characterized for their photooxidation properties. They exhibit high solubility which provides low-cost solution deposition methods. However, most of them are highly susceptible to photooxidation in solution determined with a few minutes of their half-life time under ambient conditions, practically precluding them from solution fabrication applications. Interestingly, their photooxidation stability can be significantly increased by blocking out light. The thin film transistor device for 3,4,5-trifluorophenyl-substituted pentacene (**2c**) showed the highest mobility of 1.1×10^{-2} cm^2 V^{-1} s^{-1} with the threshold voltage of 20 V when it was prepared in the dark condition.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

Solution processable organic semiconducting materials have extensively attracted research attention as components in organic thin film transistors (OTFTs) for disposable, inexpensive, large-area electronics, such as smart cards, electronic identification tags, flat-panel displays, and electronic papers [1–3]. To date, acene- and heteroacene-based organic semiconductors, such as pentacene and fused oligothiophenes, have been intensively investigated for OTFT applications [4–7]. Among them, pentacene and its derivatives have field effect mobilities over 5 cm^2 V^{-1} s^{-1} [8]. However these molecules are not very soluble in common solvents, which limit their applicability in many high-throughput coating and printing processes. Furthermore, pentacene suffers from oxidative instability by photooxidation at the C-6 and C-13 positions [9–11]. Introducing substituents at the pentacene C-6 and C-13 positions has proven to be effective for enhancing the stability of the pentacene with greatly improved carrier mobility [12–14]. Anthony and co-workers reported a class of soluble triisopropylsilylethynyl (TIPS) substituted pentacene derivatives [2]. Compared to the pentacene, the bulky TIPS substituents make the resulting pentacene derivatives very soluble in common organic solvents and afford improved photooxidation stability. Recently, a pentacene derivative with 2-thienyl group was synthesized and a hole mobility of 0.1 cm^2 V^{-1} s^{-1} was observed [15]. In this paper, we report the preparation, optical and thermal properties, and photooxidation stability of a series of substituted pentacenes with different aromatic groups such as thiophene and halogenated benzenes.

2. Experimental details

2.1. Materials

All reagents were purchased from commercial sources and solvents were purified by distillation prior to use

* Corresponding authors.
E-mail addresses: nsbaek@chemoptics.co.kr (N.S. Baek), tdkim@hnu.kr (T.-D. Kim).

http://dx.doi.org/10.1016/j.orgel.2014.11.025
1566-1199/© 2014 Elsevier B.V. All rights reserved.

unless otherwise stated. All reaction containers were flame dried under vacuum before use.

2.2. 6,13-Di(thiophen-2-yl)-6,13-dihydropentacene-6,13-diol (1a)

To a suspension of 6,13-pentacenedione (0.62 g, 2.0 mmol) in 40 mL of anhydrous THF was added 6.0 mL of a solution of thiophen-2-yl-magnesium bromide (1.0 M in THF, 6.0 mmol) under a nitrogen atmosphere at room temperature. After the suspension was dissolved, the resulting solution was refluxed with stirring for 1 h. The solution was then cooled to room temperature and poured into saturated NH_4Cl aqueous solution. The organic layer was separated and the aqueous layer was further extracted with diethyl ether. The organic layers were combined, dried with anhydrous $MgSO_4$, and concentrated under reduced pressure. The product was purified by column chromatography on silica gel with an eluent of CH_2Cl_2:hexane (3:2) to afford **1a** (Yield: 57%). ^{1}H NMR ($CDCl_3$, ppm): δ 3.50 (s, 2H), 5.77 (dd, J_1 = 3.8 Hz, J_2 = 1.0 Hz, 2H), 6,25 (dd, J_1 = 5.0 Hz, J_2 = 3.8 Hz, 2H), 6.84 (dd, J_1 = 5.0 Hz, J_2 = 1.0 Hz, 2H), 7.60 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 7.90 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 8.38 (s, 4H). ^{13}C NMR ($CDCl_3$, ppm) δ 73.0, 125.1, 126.7, 127.1, 127.5, 127.9, 128.8, 138.6, 140.9, 155.0

2.3. 6,13-Dis(3,4-dichlorophenyl)-6,13-dihydropentacene-6,13-diol (1b)

It was synthesized with a similar procedure as described for compound **1a** to afford **1b** (Yield: 46%) by using (3,4-dichlorophenyl) magnesium bromide instead of thiophen-2-yl-magnesium bromide. ^{1}H NMR ($CDCl_3$, ppm): δ 3.23 (s, 2H), 7.47–7.62 (m, 10H), 7.91 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 8.38 (s, 4H). ^{13}C NMR ($CDCl_3$, ppm) δ 78.1, 125. 2, 127.0, 127.9, 128.1, 128.7, 130.9, 131.4, 133.1, 138.5, 141.1, 145.7

2.4. 6,13-Bis(3,4,5-trifluorophenyl)-6,13-dihydropentacene-6,13-diol (1c)

It was synthesized with a similar procedure as described for compound **1a** to afford **1c** (Yield: 42%) by using (3,4.5-trifluorophenyl) magnesium bromide instead of thiophen-2-yl-magnesium bromide. ^{1}H NMR ($CDCl_3$, ppm): δ 3.27 (s, 2H), 6.99 (s, 4H), 7.64 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 7.90 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 8.40 (s, 4H) ^{13}C NMR ($CDCl_3$, ppm) δ 78.8, 118.31, 125.1, 126.9, 128.2, 137.6, 139.9, 142.3, 144.8, 150.9

2.5. 6,13-Di(thiophen-2-yl)pentacene (2a)

To a solution of **1a** (0.60 g, 1.26 mmol), sodium hypophosphite monohydrate (1.00 g, 9.43 mmol), and NaI (1.00 g, 6.67 mmol) in glacial acetic acid (7 mL) was refluxed for 30 min under nitrogen atmosphere. After cooling to room temperature, the precipitate was filtered, washed with water and methanol, and dried with reduced pressure. The resulting solid was dissolved with CH_2Cl_2 in the dark condition and purified by column chromatography on silica gel with an eluent of CH_2Cl_2:hexane (1:1) to afford **2a** (Yield: 74%). ^{1}H NMR ($CDCl_3$, ppm): δ 3.50 (s, 2H), 5.77 (dd, J_1 = 3.8 Hz, J_2 = 1.0 Hz, 2H), 6,25 (dd, J_1 = 5.0 Hz, J_2 = 3.8 Hz, 2H), 6.84 (dd, J_1 = 5.0 Hz, J_2 = 1.0 Hz, 2H), 7.60 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 7.90 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 8.38 (s, 4H). ^{13}C NMR ($CDCl_3$, ppm) δ 125.1, 125.4, 127.1, 127.5, 128.6, 129.6, 130.2, 131.2, 139.6. Anal. Calcd. for $C_{30}H_{18}S_2$: C 81.41%, H 4.10%; found: C 80.89%, H 3.96%.

2.6. 6,13-Bis(3,4-dichlorophenyl)pentacene (2b)

It was synthesized with a similar procedure as described for compound **2a** to afford **2b** (Yield: 68%). ^{1}H NMR ($CDCl_3$, ppm): δ 3.27 (s, 2H), 6.99 (s, 4H), 7.64 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 7.90 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 8.40 (s, 4H) ^{13}C NMR ($CDCl_3$, ppm) δ 126.1, 126.9, 127.7, 128.4, 128.6, 128.9, 129.9, 130.2, 132.5, 133.5, 136.2, 141.0. Anal. Calcd. for $C_{34}H_{18}Cl_4$: C 71.85%, H 3.19%; found: C 71.06%, H 3.01%.

2.7. 6,13-Bis(3,4,5-trifluorophenyl) pentacene (**2c**)

It was synthesized with a similar procedure as described for compound **2a** to afford **2c** (Yield: 75%). ^{1}H NMR ($CDCl_3$, ppm): δ 3.27 (s, 2H), 6.99 (s, 4H), 7.64 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 7.90 (dd, J_1 = 6.3 Hz, J_2 = 3.4 Hz, 4H), 8.40 (s, 4H) ^{13}C NMR ($CDCl_3$, ppm) δ 119.0, 126.6, 127.1, 128.0, 128.1, 128.9, 134.7, 136.9, 137.1, 146.9. Anal. Calcd. for $C_{34}H_{16}F_6$: C 75.84%, H 2.99%; found: C 74.76%, H 2.61%.

2.8. Characterization

^{1}H and ^{13}C NMR spectra (300 MHz) were taken on a Varian 300 spectrometer and UV/vis spectra were obtained on a Perkin-Elmer spectrophotometer. Elemental analyses were performed on Flash1112 CE Instrument. Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) were performed on a TA instruments Q50 at a ramping rate of 10 °C/min under a nitrogen atmosphere. Electrical measurements were performed at room temperature under an argon atmosphere using an HP4156C semiconductor parameter analyzer. Atomic force microscopy (AFM) was performed using a Digital Instruments Nanoscope IV operated in tapping mode (~350 kHz frequency, Si tip).

3. Results and discussion

Pentacene derivatives, **2a–c** were synthesized as shown in Scheme 1. 6,13-Pentacenequinone reacted with aromatic Grignard reagents to afford diarylpentacenediols, **1a–c** with yields of 40–60%. The pentacene derivatives were prepared by the reaction of compounds **1a–c** with $NaH_2PO_2{\cdot}H_2O$ and NaI in refluxing acetic acid. The resulting solids were purified by column chromatography under subdued safe-light to provide high yields (>70%) of **2a–c**.

Three of them did not exhibit melting points until 300 °C determined by DSC. The initial decomposition

Download English Version:

https://daneshyari.com/en/article/7701937

Download Persian Version:

https://daneshyari.com/article/7701937

Daneshyari.com