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Silyl Substituted Methanofullerenes as Electron Acceptors in Organic Photovoltaic Cells

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The electron-accepting capability of fullerenes has made them interesting materials for organic photovoltaic cells (OPVCs). In this study, we propose the new methanofullerene derivatives incorporated with trimethylsilyl moiety to increase the solubility without electron transporting property decrease. Methanofullerene acceptor materials having trimethylsilyl substituent (PCB-Sis) were synthesized from the reaction of fullerene with trimethylsilyl substituted hydrazide type derivatives, electrochemical propertie was examined by cyclicvoltametry. OPVCs fabricated by using the mixture of P3HT and mono-*adducts of PCB-Sis (Compound* **7–9***) as active layer showed 2.82% of power conversion efficiency under 100 mW/cm^2 AM1.5 simulated light after annealing at 150°C for 10 min. Also, we have synthesized* bis-*adduct type PCB-Sis as moderate yield and obtained increased* Voc *about 0.5–0.14 V from P3HT and* bis-*adduct of PCB-Sis (Compound* **10–12***) based OPVCs. Unfortunately, these* bis-*adducts show slightly lower power conversion efficiency compare to* mono-*adducts due to the numerous region-isomers of* bis-*adducts. Although it was revealed our new PCB-Sis were candidates for acceptor materials in OPVCs.*

Keywords Acceptor; C_{60}; fullerene; *n*-type; OPVCs; organic photovoltaic cells; organic semiconductor; organic solar cells; silyl

Introduction

Recently, organic photovoltaic cells (OPVCs) have attracted much attention, due to their ease of fabrication, potential for low-cost production and easy methods to produce energy from light [1]. For OPVCs, the open circuit voltage (*Voc*), the short-circuit current density (*Jsc*) and the fill factor (*FF*) are basic and important parameters, which can affect the efficiency directly. Several research groups have reported that such solution-processed organic photovoltaic cells can achieve power conversion efficiencies under standard illumination conditions (AM 1.5G, 100 mW/cm^2) in the 4–5% range with poly(3-hexylthiophene) (P3HT) [2–5] representing the cost efficient OPVCs reported to date. Nevertheless, there is still plenty of room

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Address correspondence to Sung Cheol Yoon, Korea Research Institute of Chemical Technology, Jang-dong 100, Yusung-gu Daejeon 305-600, Korea. E-mail: yoonsch@krict.re.kr to improve the efficiency of this type of bulk-heterojunction photovoltaic cell. Recently the necessity of improving the *Voc* has attracted much attention [6]. There is a need for optimizing the electronic match between the donor and acceptor component, in order to minimize unnecessary internal loss of *Voc*. Brabec *et al.* reported, within certain limits with respect to the electrodes' workfunction (i.e., as long as there are ohmic contacts at both electrodes), the *V*oc of a bulk-heterojunction PV cell scales linearly with the decrease of the first reduction potential of the acceptor [7,8]. Later, others confirmed the related relationship, between the *Voc* and the first oxidation potential of the donor material [9]. Hence, there is, within certain limits, a linear relationship between the HOMO level of donor and the LUMO level of acceptor energy difference and the *V*oc of the bulk-heterojunction device. Raising the LUMO of the acceptor, on the other hand, will directly result in a higher *Voc* without affecting the absorption of the cell. It has been shown that the second approach is theoretically more beneficial for a single-layer solar cell, and results in an estimated efficiency of 8.4% when the LUMO offset is reduced to 0.5 eV [10]. To improve *Voc*, it is necessary to decrease the HOMO energy of donor and increase the LUMO energy of the Acceptor.

During the past several years, we have already reported lots of fullerene type acceptor materials for organic photovoltaic cells to improve the OPV performance [11–13]. Now, we propose the new methanofullerene derivatives incorporated with trimethylsilyl moiety which are *mono*- and *bis*-adducts to increase the solubility without electron accepting performance decrease, as a new fullerene-based *n*-type semiconductor material. In addition, we expected that our *bis*-adducts can improve the power conversion efficiency due to the LUMO level increase.

Experimental

Materials

P3HT was purchased from Rieke Metals and C_{60} were purchased from Bucky USA. Other chemicals including solvents and reagents were purchased from Aldrich Chemicals and used without further purification.

Syntheses of PCB-Sis

Methyl 5-(4-(Trimethylsilyl)phenyl)5-oxopentanate (Compound 1). A solution of 1-bromo-4-(trimethylsilyl)benzene (5.52 g, 24.1 mmol) in dry THF (100 ml) was placed under nitrogen. Under stirring, a solution of *n*-BuLi (15 ml, 1.6 N in hexane, 24 mmol) was added dropwise while the mixture was kept at −78°C. The resulting homogeneous solution was allowed to warm up to −55°C in 30 min. Copper(I) iodide (2.38 g, 12.49 mmol) was then added at once, resulting in a creamy brown solution. The mixture was allowed to warm up to −30°C in 20 min. The obtained dark brown slurry was stirred for another 30 min, after which methyl 5-chloro-5-oxopentanoate (1.66 g, 10.1 mmol) was added, resulting in a green mixture. The mixture was allowed to warm up to 0°C in 1 h. Dry methanol (4 ml) was added, resulting in some precipitation. Aqueous ammonium chloride (50 ml) was added to the reaction mixture. The mixture was then filtered through celite. And the filtrate separated two layers of blue and green. The aqueous (blue) layer was extracted with ether (3 × 50 ml). The combined organic extracts were washed with water

(100 ml) and dried over anhydrous magnesium sulfate and concentrated *in vacuo* yielding a greenish liquid. The crude compound **1** was purified by column chromatography using the ethyl acetate and hexane to produce transparent oil.

Compound 1 (Yield: 55%): ^{1}H NMR ($CDCl_3$, ppm) δ 7.92–7.90 (d, $J = 8.1$, 2H, ArH), 7.62–7.59 (d, $J = 8.1$, 2H, ArH), 3.67 (3H, s, CH_3), 3.07–3.02 (t, $J = 7.2$, 2H, CH_2), 2.47–2.42 (t, $J = 7.2$, 2H, CH_2), 2.09–2.04 (t, $J = 7.2$, 2H, CH_2), 0.28 (9H, s, CH_3).

*3-(Trimethylsilyl)alkyl 5-Oxo-5-phenylpentanoate (Compound **2** and **3**).* Diethyl azodicarboxylate (DEAD) (9.37 mmol) was added dropwise into a solution of trimethylsilyl ethanol (7.81 mmol), triphenylphosphine (9.37 mmol), and benzoyl butyric acid (7.81 mmol) in THF (50 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 24 hr. After filtration, extraction was carried out with use of ethyl acetate. The combined organic layers were washed with water (3 × 100 ml) and then dried over anhydrous magnesium sulfate. The crude compound **2** or **3** was purified by column chromatography using the mixture of ethyl acetate and hexane to produce transparent oil.

Compound 2 (Yield: 60%): ^{1}H NMR ($CDCl_3$, ppm) δ 7.94–7.91 (d, $J = 9.0$, 2H, ArH), 7.51–7.39 (m, 2H, ArH), 4.17–4.11 (t, $J = 8.4$, 2H, CH_2), 3.04–2.99 (t, $J = 7.2$, 2H, CH_2), 2.38–2.36 (t, $J = 6.9$, 2H, CH_2), 2.05–2.01 (m, 2H, CH_2), 0.97–0.92 (t, $J = 9.0$, 2H, CH_2), 0.001 (s, 9H, CH_3).

Compound 3 (Yield: 65%): ^{1}H NMR ($CDCl_3$, ppm) δ 8.02–7.99 (d, $J = 8.7$, 2H, ArH), 7.60–7.47 (m, 3H, ArH), 4.10–4.06 (t, $J = 6.9$, 2H, CH_2), 3.13–3.08 (t, $J = 7.2$, 2H, CH_2), 2.51–2.46 (t, $J = 7.2$, 2H, CH_2), 2.15–2.10 (t, $J = 7.2$, 2H, CH_2), 1.68–1.62 (m, 3H, CH_3), 0.56–0.50 (m, 2H, CH_2), 0.04 (9H, s, CH_3).

*General Procedure of Benzoyl Butyrate P-Tosylhydrazone (Compound **4–6**).* One of Compound **1, 2**, and **3** (5.88 mmol) was mixed with *p*-touenesulfonyl hydrazide (6.47 mmol) in 30 ml MeOH. The mixture was stirred and refluxed for 5 hours. The mixture was left without heating for 4 hours and then cooled to −10°C. Compound **4, 5,** or **6** was crystallized from the mixture and collected by filtration and washed with chilled MeOH.

Compound 4 (Yield: 65%): ^{1}H NMR ($CDCl_3$, ppm) δ 9.13 (s, 1H, NH), 7.72–7.69 (d, $J = 8.4$, 2H, $ArSO_{2-}$), 7.45–7.42 (d, $J = 8.1$, 2H, ArH), 7.29–7.26 (d, $J = 8.1$, 2H, ArH), 7.08–7.05 ($J = 8.4$, 2H, $ArSO_{2-}$), 3.51 (3H, s, CH_3), 2.46–2.41 (t, $J = 8.1$, 2H, CH_2), 2.15 (s, 3H, CH_3), 2.11–2.06 (m, 2H, CH_2), 1.50–1.45 (m, 2H, CH_2), 0.03 (9H, s, CH_3).

Compound 5 (Yield: 85%): ^{1}H NMR ($CDCl_3$, ppm) δ 9.30 (s, 1H, NH), 7.93–7.90 (d, $J = 9.0$, 2H, $ArSO_{2-}$), 7.66–7.63 (m, 2H, ArH), 7.35–7.32 (m, 3H, ArH), 7.31–7.28 (d, $J = 9.0$, $ArSO_{2-}$), 4.33–4.27 (t, $J = 9.0$, 2H, CH_2), 2.66–2.60 (t, $J = 9.0$, 2H, CH_2), 2.40 (s, 3H, CH_3), 2.30–2.26 (t, $J = 6.0$, 2H, CH_2), 1.72–1.63 (m, 2H, CH_2), 1.07–1.01 (t, $J = 9.0$, 2H, CH_2), 0.001 (s, 9H, CH_3).

Compound 6 (Yield: 95%): ^{1}H NMR ($CDCl_3$, ppm) δ 9.30 (s, 1H, NH), 7.93–7.90 (d, $J = 8.4$, 2H, $ArSO_{2-}$), 7.66–7.63 (m, 2H, ArH), 7.35–7.32 (m, 3H, ArH), 7.30–7.27 (d, $J = 8.4$, $ArSO_{2-}$), 4.18–4.13 (t, $J = 7.2$, 2H, CH_2), 2.66–2.61 (t, $J = 7.8$, 2H, CH_2), 2.40 (s, 3H, CH_3), 2.33–2.29 (t, $J = 7.8$, 2H, CH_2), 1.71–1.66 (m, 4H, CH_2), 1.07–1.01 (t, $J = 8.7$, 2H, CH_2), 0.02 (s, 9H, CH_3).

*General Procedure of PCB-Sis (Benzoyl C_{61} Butyric Acid Trimethylsilyl Alkyl Ether, Compound **7–12**).* One of *p*-tosylhydrazone compounds **4**, **5**, and **6** (7.81 mmol) was dissolved in 10 mL of dry pyridine in a dried two-necked flask provided with N_2 inlet, a thermometer, and a magnetic stirring bar. Then, NaOMe (8.12 mmol) was added, and the mixture was stirred during 15 min. A solution of C_{60} (3.51 mmol) in *o*-DCB (100 mL) was added, and the homogeneous reaction mixture was stirred overnight at 70°C under argon atmosphere. The solution was heated to reflux, and the reaction was allowed to continue overnight again. *Bis*-adducts of PCB-Sis are normally obtained as by-product of the preparation of *mono*-adduct of PCB-Sis. The crude compound was purified and separated by column chromatography using the mixture of ethyl acetate and hexane. The solution was concentrated *in vacuo*, redissolved in a minimal amount of dichloromethane, and transferred to a centrifuge tube. The product was precipitated with MeOH, centrifuged, and decanted. The product was treated with MeOH several times in the same manner and washed with a mixture solution (MeOH:Hexane, 5:1% v/v).

Compound 7 (Yield: 25%): ^{1}H NMR ($CDCl_3$, ppm) δ 7.89–7.86 (d, $J = 8.1$, 2H, ArH), 7.68–7.66 (d, $J = 8.1$, 2H, ArH), 3.68 (s, 3H, CH_3), 2.92–2.89 (t, $J = 8.1$, 2H, CH_2), 2.55–2.50 (t, $J = 7.5$, 2H, CH_2), 2.21–2.15 (m, 2H, CH_2), 0.35 (s, 9H, CH_3).

^{13}C NMR ($CDCl_3$, 75.49 MHz): δ 174.50, 149.82, 146.91, 146.21, 146.05, 145.80, 145.68, 145.52, 145.44, 145.02, 144.78, 144.08, 143.94, 143.15, 141.99, 139.03, 138.75, 134.37, 132.26, 102.43, 80.90, 52.97, 52.65, 34.92, 34.72, 23.40, 0.02.

Compound 8 (Yield: 40%): ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.94–7.92 (d, $J = 6.0$, 2H, ArH), 7.57–7.47 (m, 3H, ArH), 4.19–4.14 (d, $J = 9.0$, 2H, CH_2), 2.94–2.88 (t, $J = 6.0$, 2H, CH_2), 2.52–2.47 (t, $J = 7.4$, 2H, CH_2), 2.21–2.16 (m, 2H, CH_2), 1.00–0.94 (t, $J = 8.4$, 2H, CH_2), 0.04 (s, 9H, CH_3).

^{13}C NMR ($CDCl_3$, 75.49 MHz): δ 150.29, 149.29, 147.32, 146.64, 146.47, 146.11, 145.93, 145.45, 144.44, 144.38, 143.65, 143.59, 142.44, 142.20, 139.51, 139.02, 133.55, 129.88, 81.37, 64.20, 53.38, 35.78, 35.17, 23.86, 18.81, 0.04.

Compound 9 (Yield: 45%): ^{1}H NMR ($CDCl_3$, ppm) δ 7.94–7.92 (d, $J = 6.9$, 2H, ArH), 7.57–7.47 (3H, m, ArH), 4.05–4.00 (t, $J = 7.2$, 2H, CH_2), 2.94–2.89 (t, $J = 8.1$, 2H, CH_2), 2.55–2.50 (t, $J = 7.5$, 2H, CH_2), 2.21–2.16 (m, 2H, CH_2), 1.63–1.59 (m, 2H, CH_2), 0.51–0.45 (t, $J = 8.7$, 2H, CH_2), 0.004 (s, 9H, CH_3).

^{13}C NMR ($CDCl_3$, 75.49 MHz): δ 174.79, 150.55, 149.56, 147.60, 146.92, 146.88, 146.82, 146.39, 146.15, 145.49, 144.76, 144.72, 144.66, 143.97, 143.91, 143.84, 139.78, 139.29, 133.82, 130.16, 81.64, 68.98, 53.64, 35.87, 35.42, 24.99, 24.15, 14.22, 0.02.

Compound 10 (Yield: 20%): ^{1}H NMR ($CDCl_3$, ppm) δ 8.11–7.54 (m, 4H, ArH), 3.70–3.62 (m, 3H, CH_3) 2.77–2.01 (m, 6H, CH_2), 0.41–0.27 (m, 9H, CH_3).

Compound 11 (Yield: 40%): ^{1}H NMR ($CDCl_3$, ppm) δ 8.16–7.33 (m, 5H, ArH), 4.23–4.08 (m, 2H, CH_2), 2.78–2.05 (m, 6H, CH_2), 1.03–0.89 (m, 2H, CH_2), 0.06–0.00 (m, 9H, CH_3).

Compound 12 (Yield: 40%): ^{1}H NMR ($CDCl_3$, ppm) δ 8.17–7.37 (m, 5H, ArH), 4.10–3.96 (m, 2H, CH_2), 2.81–2.05 (m, 6H, CH_2), 1.69–1.61 (m, 2H, CH_2), 0.51–0.43 (m, 2H, CH_2), 0.02–0.00 (m, 9H, CH_3).

Electrochemical and Photophysical Properties of PCB-Sis

The cyclicvoltametry (BAS 100) was performed with a solution of tetrabutylammonium tetrafluoroborate ($Bu_4N^+BF_4^-$, 0.10 M) as the electrolyte and material (10^{-3} M) in *o*-dichlorobenzene at a scan rate of 100 mV/s at room temperature under argon atmosphere. A glassy carbon electrode (0.3 mm diameter) was used as the working electrode.

A Pt and an Ag/Ag^+ electrode were used as the counter electrode and reference electrode, respectively.

Device Fabrications

The organic photovoltaic cells were built in sandwiched structure between a transparent anode and cathode by spin-coating. The anode consisted of glass substrates pre-coated with indium tin oxide (ITO), modified by spin-coating PEDOT/PSS (Bytron P, AI4083) layer (40 nm) followed thermal treatment at 200°C for 5 min after UV/ozone on the surface of ITO, and then a blend of P3HT and one of new compound mixture in *o*-dichlorobenzene was spin-coated. Metal cathode was deposed by thermal evaporation consisted with LiF and Al approximately 0.5 Å and 130 nm thick. Finally, all devices were encapsulated with glass cap containing moisture capture materials, calcium oxide. Additional thermal annealing was proceeded at 150°C for 10 minutes.

J-V Measurements

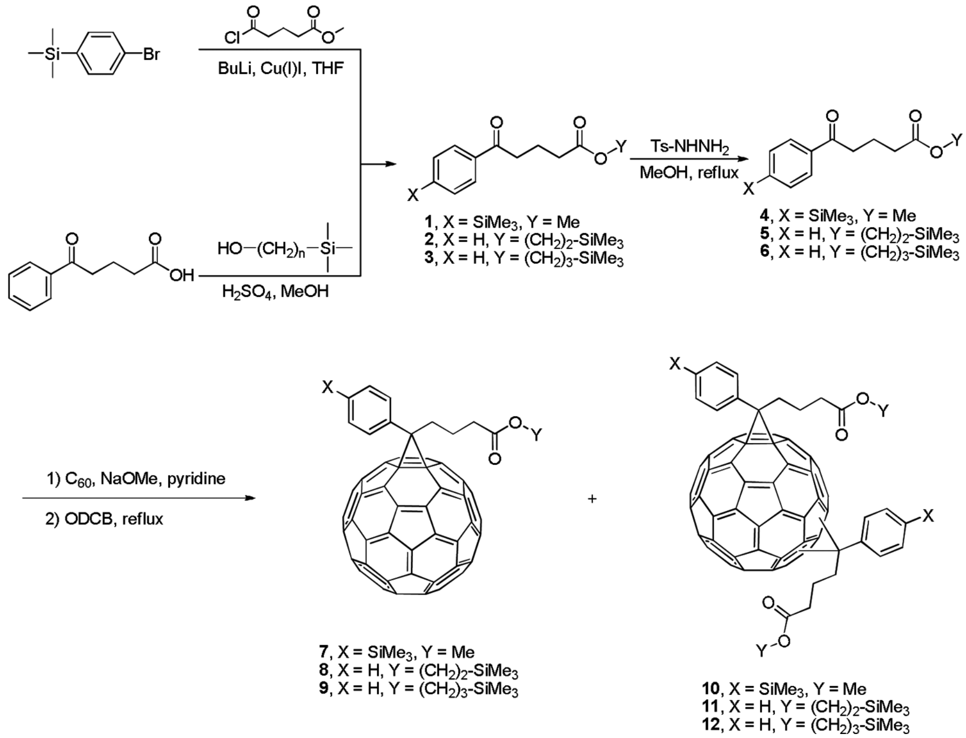
Photocurrent-voltage curve measurements of each device were performed at room temperature. The current-voltage (*I-V)* curves of the devices were obtained using a Keithley 2400 Source Measure Unit under AM 1.5 simulated light (ORIEL 300 W Xenon lamp). The intensity of light (100 mA/cm^2) from the illumination source was confirmed by using a standard silicon photodiode (BS520, Bunkoh-Keiki).

Results and Discussion

Syntheses and Characterizations of PCB-Sis

The synthetic scheme of trimethylsilyl-substituted [60]methanofullerene derivatives (PCB-Sis, compound **7**–**12**) is depicted in Scheme 1. The methyl 5-(4-(trimethylsilyl)-phenyl)-5-oxopentanate (**1**) was prepared by Friedel-Crafts acylation of 1-bromo-4-(trimethylsilyl)-benzene with *n*-BuLi (55%). The benzoylbutyric acid was then converted to the compound **2** and **3** in trimethylsilyl ethanol, trimethylsilyl butanol under Fischer esterification conditions (70%). The syntheses of PCB-Sis (compound **7**–**9**) were carried out by the Wudl-Hummelen approach [14]. Condensation of compound **1**–**3** with *p*-tosylhydrazide in methanol afforded the corresponding *p*-tosylhydrazone compound **4**–**6**. After sequential treatment with sodium methoxide in pyridine and fullerene C_{60} in refluxing *o*-dichlorobenzene, *mono*-adducts of PCB-Sis (compound **7**–**9**) were obtained with the yield from 30% to 40%.

Although both [6,6] and [5,6] isomers could be expected from the cycloaddition reaction, the high temperature allowed the isolation of the thermodynamically more stable [6,6] isomer, exclusively, as determined by ^{1}H-NMR. Synchronously, *bis*-adducts (compound **10**–**12**) can be produced with the proceeding of the reaction (yield: 20–40%), which could be separated using standard column chromatography. In addition, we can confirm that *bis*-adducts contain of a number of region-isomers by ^{1}H-NMR and FAB-Mass spectroscopy. The ^{1}H NMR spectra of *mono*- (**7**) and *bis* TMS-PCBM (**10**) are shown in Figure 1. From the ^{1}H NMR measurements, the methylene protons of substituents show widely split peaks around 0.08–0.14 ppm,



Scheme 1. Syntheses of PCB-Sis (Compounds **7**–**12**).

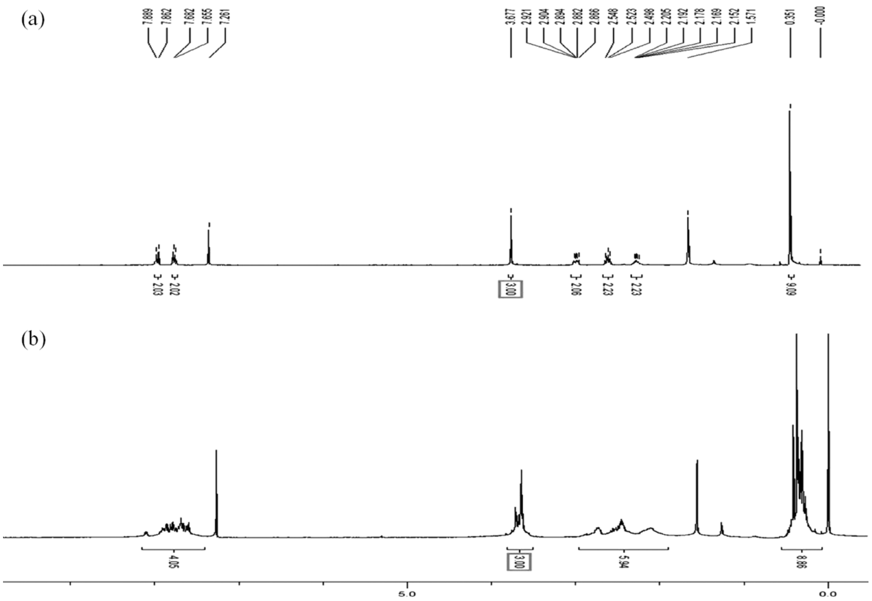


Figure 1. ^{1}H NMR spectra of *mono-* (**7**) and *bis* TMS-PCBM (**10**).

which proved the presence of at least 10 methoxy resonace signals indicating that the bis-adducts consisted of a much more complex mixture of isomer. In addition, all of our PCB-Sis (Compound 7–12) show much higher solubility in common organic solvents, such as chloroform, chlorobenzene, *o*-dichlorobenzene, and so on. Generally, the purity of organic semiconductor is very important to perform the charge transportation.

Electrochemical Properties of PCB-Sis

The electrochemical properties of PCB-Sis were studied by cyclic voltammetry (CV) at room temperature in *o*-DCB solution. Each of new methanofullerenes shows similar cyclic voltammograms of thee reversible reductive potentials ranged from 0.0 V to −2.4 V with PCBM. Tree representative curves were chosen to distinguish clearly reduction potential as shown in Figure 2 and Table 1.

From these experiments, the first reductive potentials of all *mono*-adducts of PCB-Sis (Compound **7**–**10**) show similar with that of PCBM. On the other hand, the first reductive potentials of *bis*-adducts (compound **10**–**12**) show much more negative than that of PCBM. This means that *bis*-adducts of PCB-Sis have much higher LUMO energy level compare to *mono*-adducts of PCB-Sis and PCBM by about 0.13–0.17 V. It can be concluded that we can obtain highly efficient OPVCs due to the *Voc* improvement.

The Performances of Organic Solar Cells

The organic photovoltaic cells were fabricated using one of newly synthesized PCB-Sis as electron acceptor with conventional donor polymer (regioregular P3HT) as a donor material. The *J-V* characteristics of OPVCs are shown in Figure 3 and *Voc, Jsc, FF,* and power conversion efficiency (*PCE*) were summarized in Table 2. The device performance were measured under 100 mW/cm^2 AM 1.5 simulated light illumination after annealing at 150°C for 10 min.

Power conversion efficiency of each device is recorded from 0.57 to 2.82%. And open circuit voltage (*Voc*) of each device is recorded from 0.64 to 0.78 V. As shown in the previous Cyclic Voltammetry experiment, we have already confirmed that *bis*-adducts have much higher LUMO level than *mono*-adducts. However, devices using *bis*-PCB-Sis as acceptor materials show lower power conversion efficiency (1.53%) than OPVCs using *mono*-PCB-Sis as acceptor materials. We expected that the regio-isomers of *bis*-adducts have various electronic states and this mixture may influence on the electron transporting performance of acceptor molecules from donor-acceptor junction to electrode. Actually, the lower power conversion efficiency of OPV using *bis*-adducts as acceptors is resulted from the lower current density and fill factor. This means a lot of photo-generated charges are dissociated in the channel of the *n*-type materials. Therefore, it is very important to purify the acceptor molecules because the purity of *bis*-adducts is a key factor to determine the photovoltaic property. And now, we are studying to develop the purification process of *bis*-PCB-Sis to increase the power conversion efficiency in OPVCs.

In conclusion, we are designed and synthesized a series of novel fullerene derivatives (*mono*- and *bis*-PCB-Sis, compound **7**–**12**) in order to minimize the energy loss in the electron transfer from the donor to the acceptor material in bulk

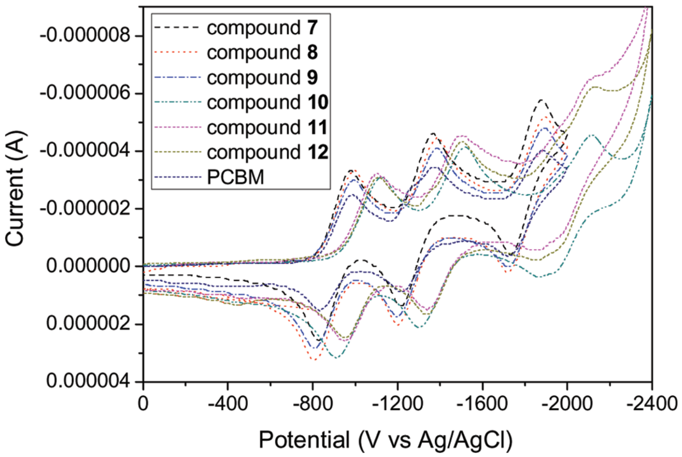
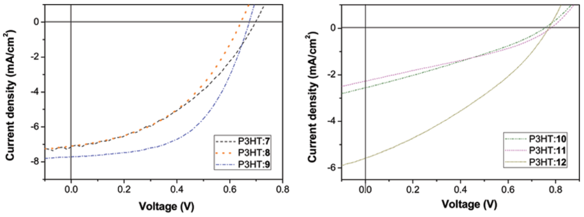


Figure 2. Cyclic voltamograms of PCB-Sis and PCBM.

Table 1. Electrochemical properties and energy levels of the PCB-Sis and PCBM

Compounds	$E^1_{1/2}$ reduction (V)	LUMO (eV)
7	−0.90	−3.65
8	−0.90	−3.65
9	−0.90	−3.65
10	−1.07	−3.48
11	−1.03	−3.52
12	−1.03	−3.52
PCBM	−0.90	−3.65

*Experimental conditions: Bu_4NF_4Br (0.1 M) as the supporting electrolyte, ODCB as the solvent, 50 mV/s scan rate.



(a) (b)

Figure 3. *J-V* characteristics of ITO/PEDOT:PSS/P3HT:PCB-Sis/LiF/Al after annealing condition [PCB-Sis: (a) *mono*-adduct; (b) *bis*-adduct].

Table 2. Photovoltaic properties of OPVC after annealing at 150°C for 10 min using one of new compounds as acceptor materials

Acceptors	*Voc* (V)	*Jsc* (mA/cm^2)	*FF* (%)	η (%)
7	0.70	7.15	40.8	2.03
8	0.64	7.11	43.9	2.01
9	0.67	7.72	54.3	2.82
10	0.75	2.56	29.8	0.57
11	0.78	2.27	35.5	0.58
12	0.77	5.86	34.0	1.53

*ITO/PEDOT-PSS/P3HT:Acceptor/LiF/Al.
*Under AM 1.5 simulated light illumination (100 mW/cm^2).

heterojunction solar cells. The additional functionalization of the fullerene cage in *bis*-adduct was shown to have little negative influence on the charge-carrier properties of the fullerene. As predicted, the higher LUMO resulted in a significantly enhanced *Voc* when used in combination with P3HT. *Bis*-PCB-Sis have higher LUMO energy level and *Voc* compared to those of *mono*-PCB-Sis by about 0.1 V. The highest power conversion efficiency of 2.82% can be obtained from ITO/PEDOT:PSS/P3HT:compound **8**/LiF/Al device after annealing at 150°C for 10 min. Even if OPV using *bis*-PCB-Sis as acceptor materials have advantage of high *Voc* value (0.78 V), device performance was slightly lower than the devices using *mono*-PCB-Sis as acceptor materials due to the regio-isomerization of *bis*-adducts. Now, we are trying to increase the purity of *bis*-PCB-Sis and additional improvement using *bis*-PCB-Sis as acceptor materials will be reported in the end of this year.

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