

Supporting Information

Donor-Acceptor Interface Stabilizer Based on Fullerene Derivatives toward Efficient and Thermal Stable Organic Photovoltaics

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In the previous research, we tried to employ PCB-C8oc as an acceptor and made P3HT: PCBM, P3HT: PCB-C8oc two kinds devices. During this process, we found an interesting phenomenon that the P3HT: PCB-C8oc film showed more deep amaranthine color than the P3HT: PCBM film before annealing, which was similar to situation of P3HT stacking. So the UV-absorption spectrum and X-ray diffraction (XRD) were employed to detect P3HT crystallinity variations in the blends containing different amounts of PCB-C8oc without thermal annealing (Figure S4). The P3HT absorption peaks at 506, 550, and 603 nm strengthened with the higher proportion of PCB-C8oc. Meanwhile, intermolecular interactions between P3HT and PCB-C8oc caused a red shift of the optical absorption of P3HT, which resulted in a better overlap with the solar emission. And the increasing crystallization peak at $2\theta=5.4$ also demonstrated that the import of PCB-C8oc can accelerate the stacking of P3HT. So we knew that PCB-C8oc can promote the orderly arrangement and compact stack of P3HT.

As is known to all, P3HT is a kind of semi-crystalline polymer. P3HT molecule could produce strong thermal motion because hexyl side chain of one molecule had a strong intermolecular interactions (alkyl-alkyl interaction) with adjacent hexyl side chain of another P3HT molecule, which induced the orderly arrangement of polymer chain segment and compact stack of P3HT under appropriate thermal annealing (Figure S5a). Analogously, the principle that PCB-C8oc promoting the stack of P3HT

can be explained by the intermolecular alkyl-alkyl interaction between PCB-C8oc's octyl groups and P3HT's hexyl side chains (Figure S5b).

So we fabricated devices of 0%, 5%, 10%, 20% without thermal annealing before evaporating cathode. From the J-V curve (Figure S3), it was obviously that 10% and 20% devices showed little better PCE than 0% devices (Table S2). This phenomenon implied that the interaction between alkyl chains of P3HT became stronger. The active layer was spined quickly, so it was hard for the special semi-crystalline P3HT to get a tight stacking. While the import of PCB-C8oc promote the ordered arrangement of polymer chain. The interaction between octyl groups in PCB-C8oc and hexyl groups in P3HT induced relatively stacking of the polymer.

Specific Synthetic procedures.

Synthesis of PCBA. 500 mg [6, 6]-Phenyl-C61-butyricacidmethylester (PCBM) with 100 ml chlorobenzene, 50 ml hydrochloric acid and 20 ml glacial acetic acid were refluxed in a two-necked flask at the temperature of 130 °C. The reaction process was monitored by Thin-Layer Chromatography, when the brown spot of PCBM disappeared, the reaction could stop. Then the redundant solvent was removed by pressure distillation. After that, the material was washed in methylbenzene, diethyl ether, Methyl alcohol in sequence by ultrasound. Repeated that washing process until get transparent cleaning solution, and solid remaining was the target material.

Synthesis of BC8oc. 3,5-dihydroxy-benzyl alcohol (1.68 g, 12 mmol), n-octyl bromide (6.25 ml, 36 mmol), potassium carbonate (4.98 g, 36 mmol) and 18-crown-6 (0.316 g, 1.2 mmol) were injected into 50ml purified acetone. After a two-day reflux with nitrogen protection, 10% vol 10% hydrochloric acid solution (10% vol. HCl) was injected to terminate the reaction. Then the reaction liquid was extracted with chloroform for three times, the coalescent organic phase was sequentially washed by water, diluted hydrochloric acid, saturated salt solution. At last, organic liquid was drying with Magnesium sulfate anhydrous and refined by silica-gel column chromatography (eluant: ethyl acetate/ petroleum ether = 1/19 in volume ratio) for separation to get the colorless oily product (2.58 g, 60%). ¹H NMR was showed in Fig S7. ¹HNMR(400 Hz, CDCl₃):δ 6.49 (s, 2H), 6.37 (s, 1H), 4.61 (s, 2H), 3.94-3.92 (t, 4H), 1.78-1.73 (m, 4H), 1.45-1.41 (m, 4H), 1.35-1.30(m, 16H), 0.89-0.87(t, 6H).MS m/z (APCI) : 364.7(M⁺).

Synthesis of PCB-C8oc. PCBA (200 mg, 0.22 mmol), BC8oc (120 mg, 0.33 mmol), 4-dimethylaminopyridine (DMAP, 26.8 mg, 0.24 mmol) were added into 20 ml O-dichlorobenzene without water, and then Dicyclohexylcarbodiimide (DCC) which dissolved in anhydrous O-dichlorobenzene in advance was added dropwise. After stirring at room temperature for 3 days, removing solvent and using silica-gel column chromatography (eluant: methylbenzene/ petroleum ether = 2/1 in volume ratio) for separation to get dark brown and black solid. The solid was washed and sequentially fractionated by Soxhlet extraction with methanol, hexane and

trichloromethane. The solid that dissolved in the trichloromethane extraction solution was final target product (134 mg, 48%). ^1H NMR was showed in Fig S8. ^1H NMR(400 Hz, CDCl_3): δ 7.92-7.91 (d, 2H), 7.55-7.46 (m, 3H), 6.45 (s, 2H), 6.38 (s, 1;1H), 5.03 (s, 2H), 3.92-3.89 (t, 4H), 2.93-2.90 (t, 2H), 2.59-2.57 (t,2H), 2.22-2.19 (m, 2H),1.76-1.72 (m, 4H), 1.44-1.40 (m, 4H), 1.34-1.25 (m, 16H) , 0.89-0.87 (t, 6H).

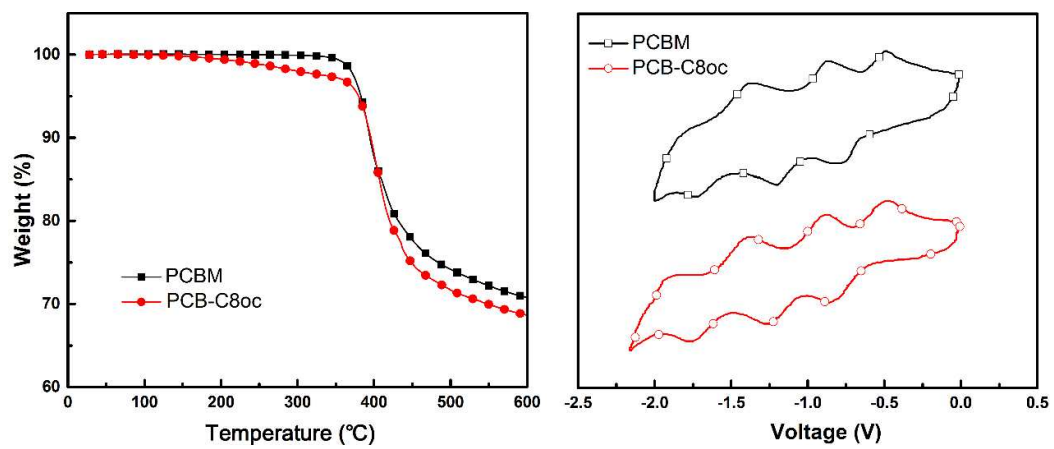


Figure S1. Thermogravimetric analysis (left) and CV curves (right) of PCBM and PCB-C8oc.

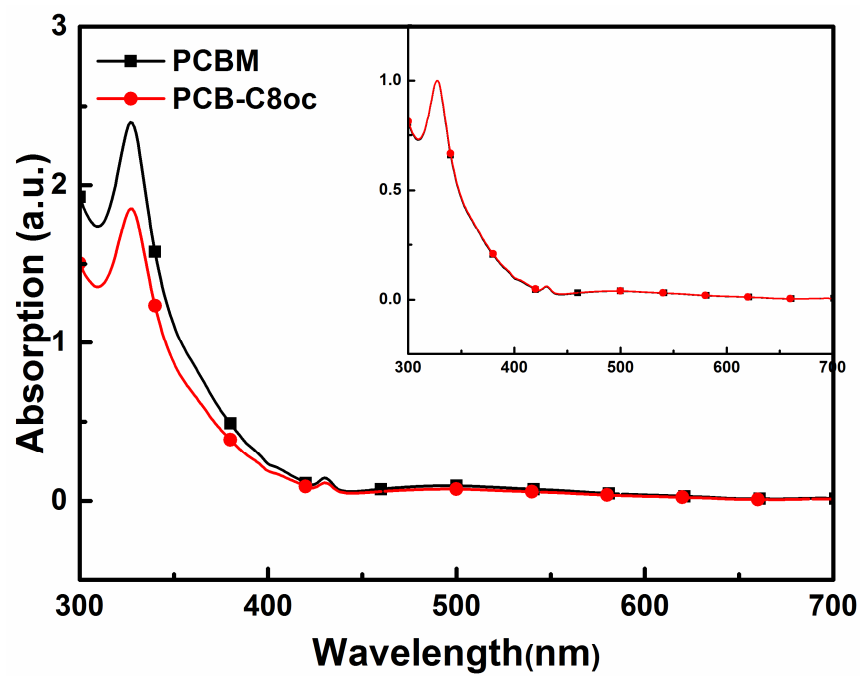


Figure S2. Absorption spectra of PCBM and PCB-C8oc films, the right one is the normalized curve.

Table S1. Photovoltaic parameters of P3HT: PCBM and P3HT: PCB-C8oc blends.

Devices	Time	Jsc (mA/cm ⁻²)	Voc (V)	FF (%)	PCE (%)
0%	15min	9.52	0.625	60.87	3.63
100%	15min	7.23	0.623	47.83	2.15

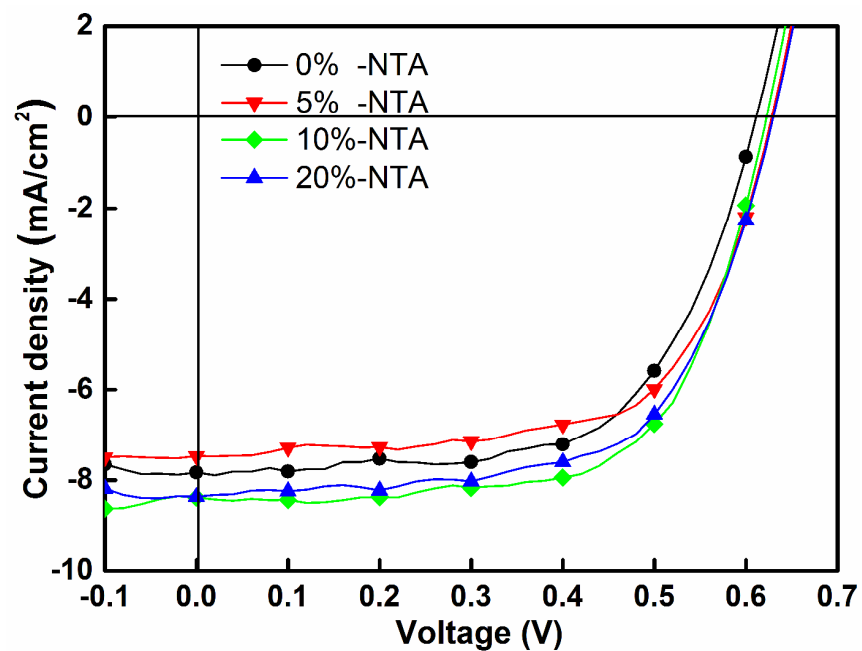


Figure S3. J-V curves of different content of PCB-C8oc devices without annealing.
(P3HT system)

Table S2. Photovoltaic parameters of different content of PCB-C8oc devices without annealing. (P3HT system)

Devices	Time	Jsc (mA/cm ⁻²)	Voc (V)	FF (%)	PCE (%)
0%	0min	7.76	0.615	61.54	2.94
5%	0min	7.47	0.628	64.86	3.04
10%	0min	8.38	0.623	65.80	3.43
20%	0min	8.36	0.630	63.61	3.35

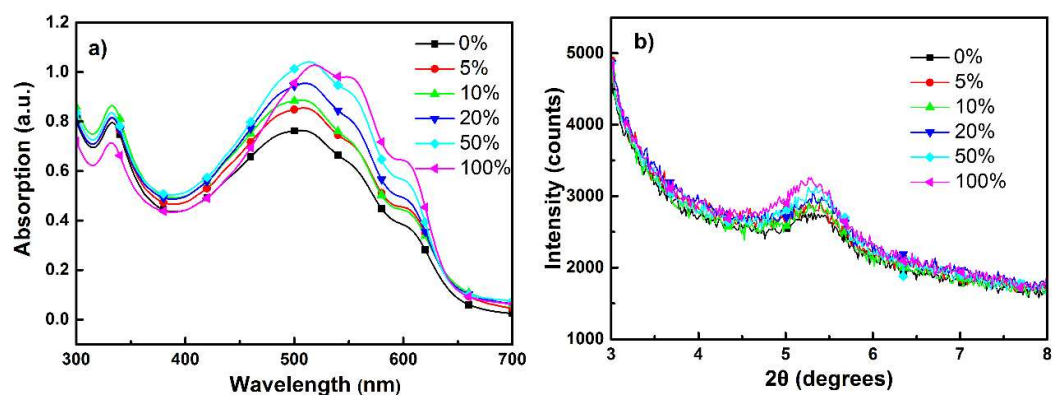


Figure S4. a) Absorption spectra and b) XRD of different content of PCB-C8oc in P3HT: PCBM: PCB-C8oc films without annealing.

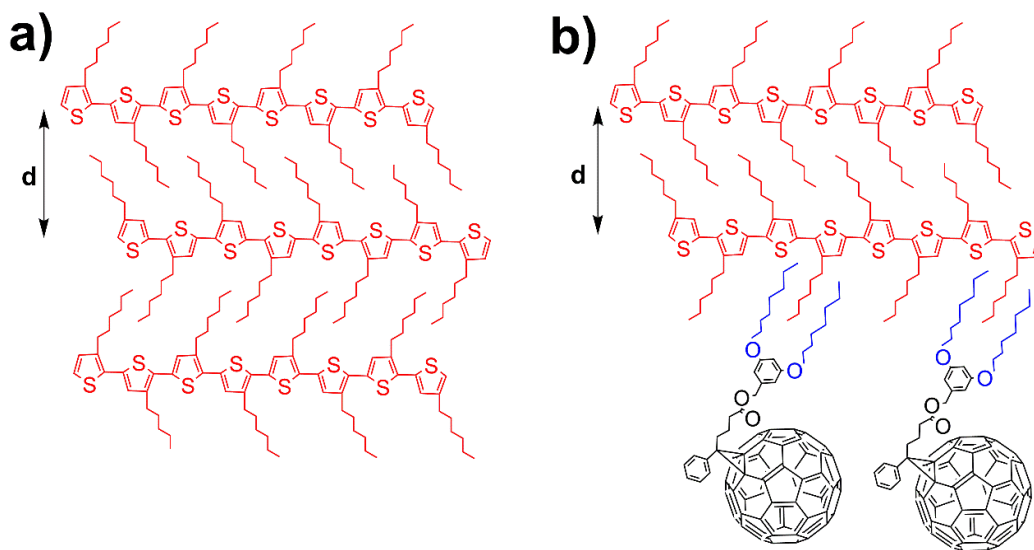


Figure S5. a) The stacking of P3HT, b) The pathway of PCB-C8oc that induce P3HT to stacking.

Table S3. Photovoltaic parameters of different content of PCB-C8oc devices without annealing (PTB7: PCBM: PCB-C8oc system).

Devices	Time	Jsc	Voc	FF	PCE
	min	(mA/cm ⁻²)	(V)	(%)	(%)
0%	0	13.26	0.743	68.54	6.76
5%	0	13.03	0.743	69.14	6.70
10%	0	11.78	0.748	64.97	5.72
20%	0	11.47	0.750	64.28	5.53

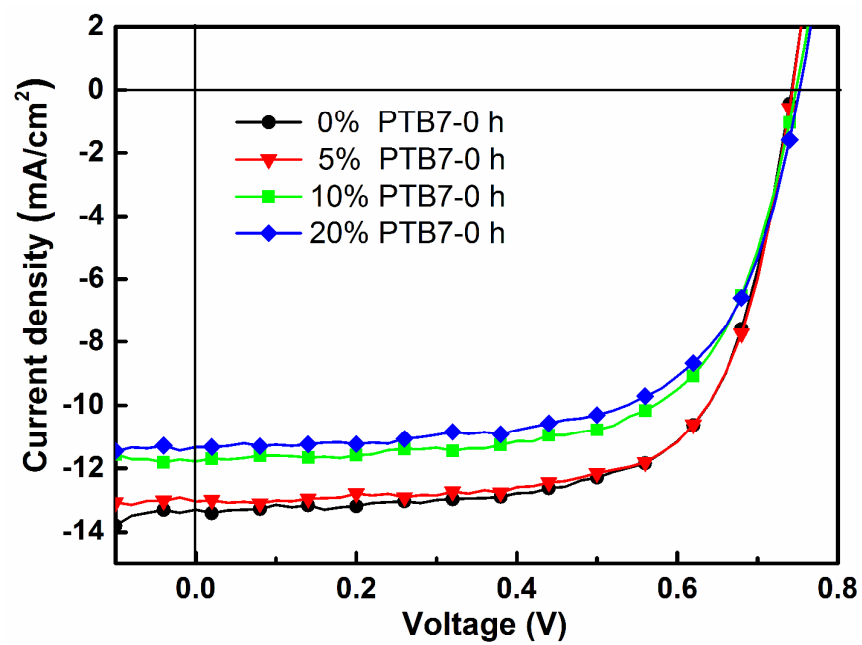


Figure S6. J-V curves of different content of PCB-C8oc devices without annealing.
(PTB7 system)



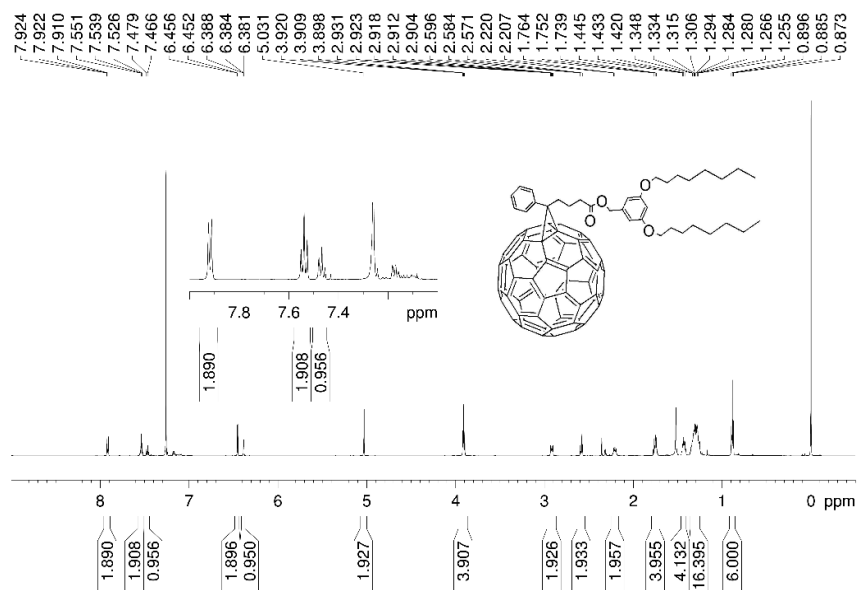


Figure S8. ^1H NMR of PCB-C8oc.