

## Supporting Information

### Semi-Transparent Low-Donor Content Organic Solar Cells Employing Cyclopentadithiophene-Based Conjugated Molecules

Jungho Lee<sup>a,†</sup>, Jeff L. Hernandez<sup>b,†</sup>, Ian Pelse<sup>b</sup>, John R. Reynolds<sup>b\*</sup>, Changduk Yang<sup>a\*</sup>

†These authors contributed to the work equally.

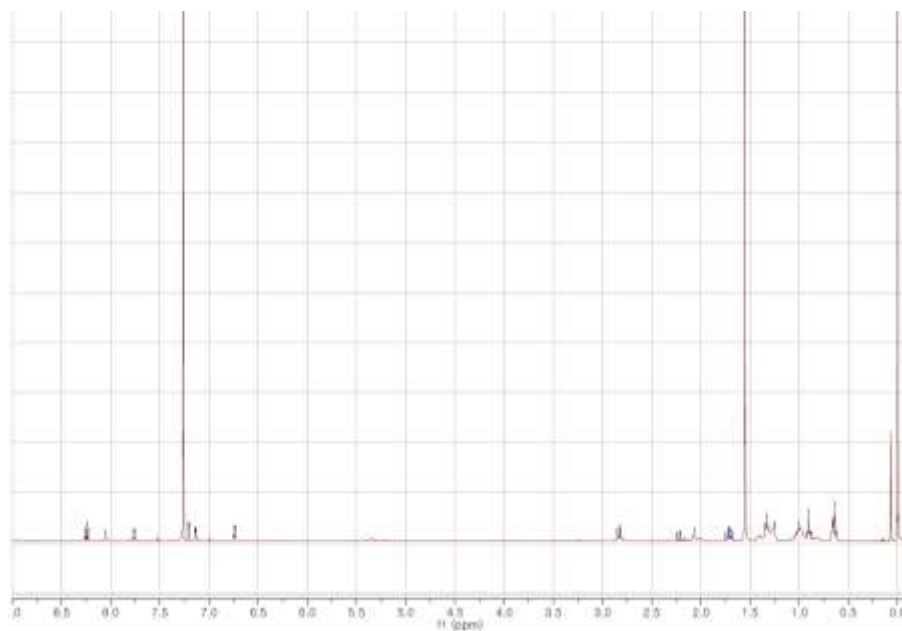
<sup>a</sup>Department of Energy Engineering, School of Energy and Chemical Engineering, Perovtronics Research Center, Low Dimensional Carbon Materials Center, Ulsan National Institute of Science and Technology (UNIST), 50 UNIST-gil, Ulju-gun, Ulsan 44919, South Korea. \*Email: Yang@unist.ac.kr

<sup>b</sup>School of Chemistry and Biochemistry, School of Materials Science and Engineering, Center for Organic Photonics and Electronics, Georgia Tech Polymer Network, Georgia Institute of Technology, Atlanta, Georgia 30332, United States. \*Email: [reynolds@chemistry.gatech.edu](mailto:reynolds@chemistry.gatech.edu).

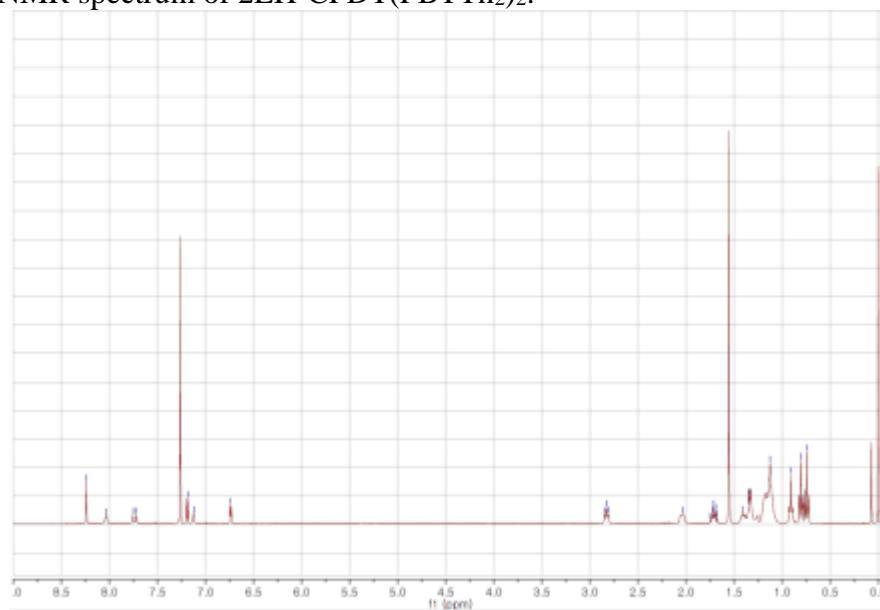
### Table Contents

1. <sup>1</sup>H NMR spectra of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>
2. UV-Vis absorption spectra of blend films
3. The UPS spectra of neat films
4. DFT calculated geometry
5. OSCs characteristics
6. 1d GIWAXS line cuts in the  $q_z$  and  $q_{xy}$  directions

- $^1\text{H}$  NMR spectra of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>.

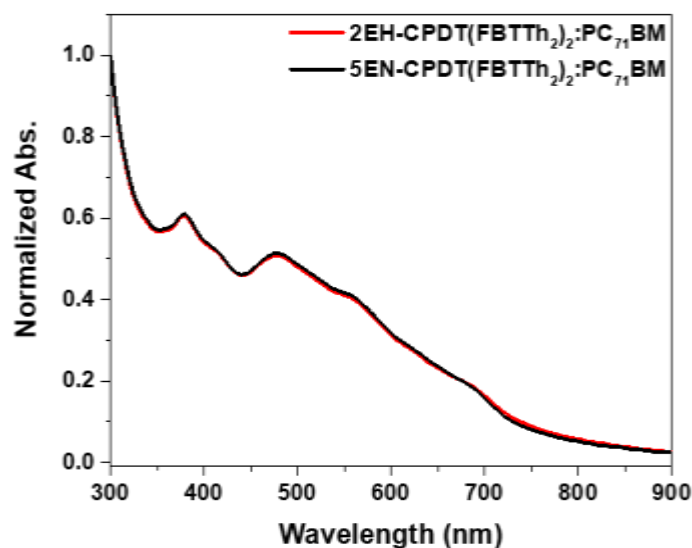


**Fig. S1.**  $^1\text{H}$  NMR spectrum of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>.



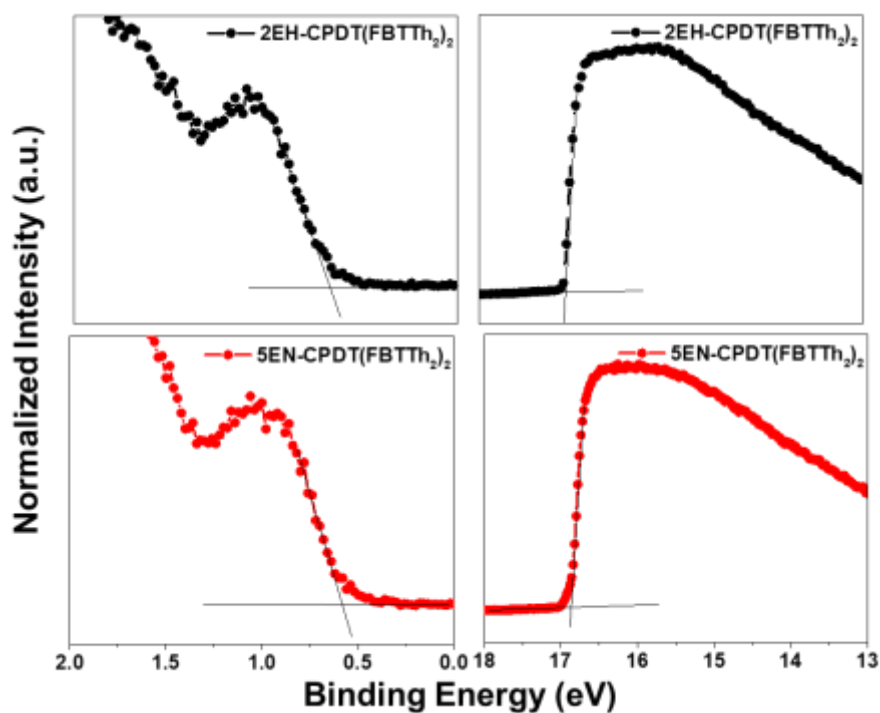
**Fig. S2.**  $^1\text{H}$  NMR spectrum of 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>.

2. UV-Vis absorption spectra of blend films



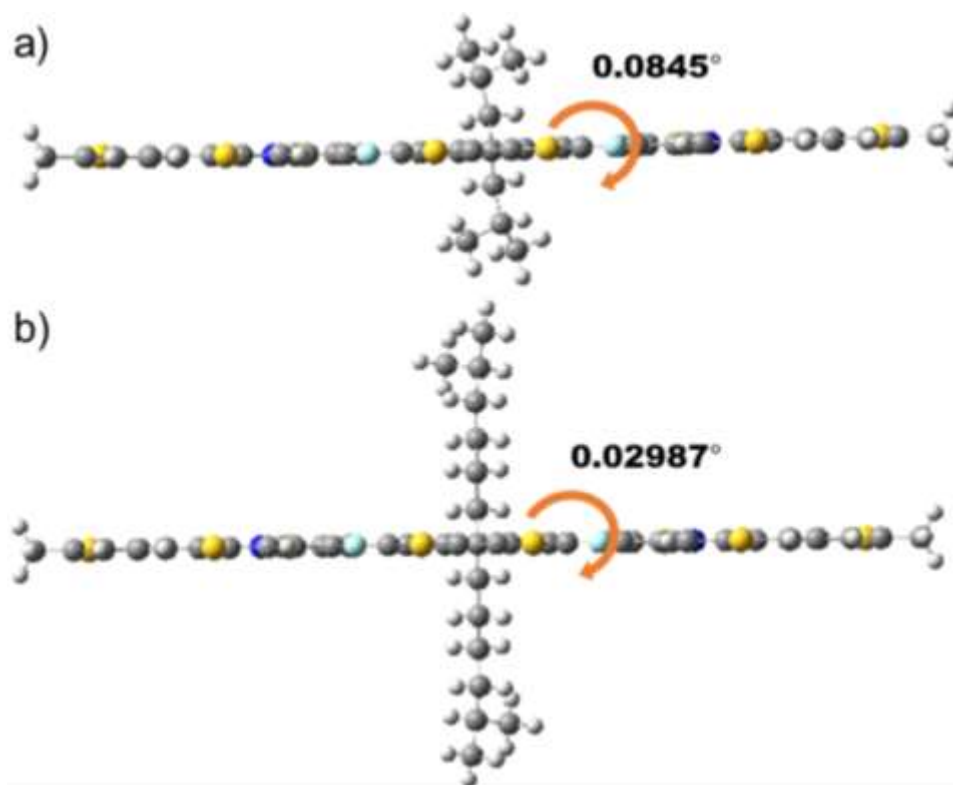
**Fig. S3.** UV-Vis absorption spectra of BHJ films of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM (1:9) and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM (1:9).

3. The UPS spectra of neat films



**Fig. S4.** Ultraviolet photoelectron spectra of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> using HeI emission ( $h\nu = 21.2$  eV) as a light source. The calculated HOMO levels of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> are  $-5.02$  eV and  $-4.92$  eV, respectively.

#### 4. DFT calculated geometry



**Fig. S5.** DFT calculated geometry (side view) of a) 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and b) 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>.

#### 5. The OSCs characteristics

**Table S1.** The OSCs characteristics composed of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM (1:9) with post treatment.

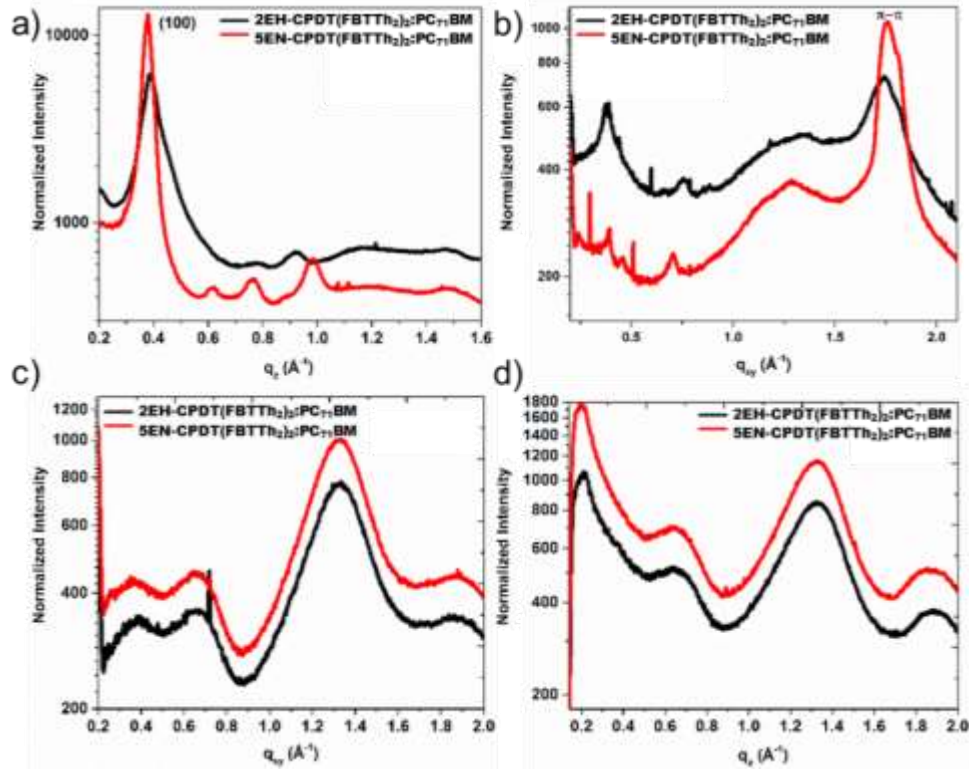
<i>2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM (1:9)</i>	<i>J<sub>sc</sub> (mA cm<sup>-2</sup>)</i>	<i>V<sub>oc</sub> (V)</i>	<i>FF (%)</i>	<i>PCE (%)</i>
<i>Annealing at 150 °C for 10 min</i>	2.88	0.61	24.7	0.43
<i>0.5% DIO</i>	1.68	0.60	32.0	0.32
<i>1% DIO</i>	0.51	0.29	31.7	0.05

**Table S2.** The OSC characteristics with different ratio composition of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> with PC<sub>71</sub>BM.

<i>D:A Ratio</i>	<i>2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM</i>				<i>5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM</i>			
	<i>J<sub>sc</sub> (mA cm<sup>-2</sup>)</i>	<i>V<sub>oc</sub> (V)</i>	<i>FF (%)</i>	<i>PCE (%)</i>	<i>J<sub>sc</sub> (mA cm<sup>-2</sup>)</i>	<i>V<sub>oc</sub> (V)</i>	<i>FF (%)</i>	<i>PCE (%)</i>
5:5	4.85	0.82	41.4	1.64	N/A <sup>a</sup>	N/A <sup>a</sup>	N/A <sup>a</sup>	N/A <sup>a</sup>
4:6	4.64	0.75	37.9	1.32	1.68	0.58	14.5	0.13
3:7	4.87	0.79	41.0	1.57	1.83	0.55	13.3	0.13
2:8	5.30	0.79	42.2	1.76	2.10	0.62	13.6	0.17
1:9	9.50	0.81	41.4	3.19	6.29	0.62	39.1	1.52
1:10	7.00	0.77	45.1	2.43	5.00	0.60	38.2	1.15
1:13	5.14	0.63	27.5	0.91	1.23	0.61	20.8	0.16

<sup>a</sup>The film formation was not properly formed for OSCs.

6. 1d GIWAXS line cuts in the  $q_z$  and  $q_{xy}$  directions



**Fig. S6.** 1d GIWAXS line cuts in the a)  $q_{xy}$  and b)  $q_z$  direction for neat 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> films and line cuts in the c)  $q_{xy}$  and d)  $q_z$  direction for 1:9 weight ratio of blend films 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub>:PC<sub>71</sub>BM.

**Table S3.** GIWAXS parameters of 2EH-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> and 5EN-CPDT(FBTTh<sub>2</sub>)<sub>2</sub> films. Lamellar and  $\pi$ - $\pi$  stacking distances were determined using  $2\pi/q$ , and crystal coherence length (CCL) was determined using  $2\pi/\text{FWHM}$ .

	$q_{xy}$			$q_z$		
	Lamellar stacking (Å)	$\pi$ - $\pi$ stacking (Å)	CCL ( $\pi$ - $\pi$ peak nm)	Lamellar stacking (Å)	$\pi$ - $\pi$ stacking (Å)	CCL (Lamellar peak nm)
2EH-CPDT(FBTTh <sub>2</sub> ) <sub>2</sub>	16.8	3.6	1.8	16.2	N/A	7.7
5EN-CPDT(FBTTh <sub>2</sub> ) <sub>2</sub>	16.0	3.6	3.9	16.6	N/A	16.9