

Electronic Supporting Information
For

**Investigation of Substitution Effect on Poly(bis-3,4-
ethylenedioxythiophene methine)s through Solid State
Polymerization**

Kai Peng, Tong Pei, Zhaoxiang Li, Lili Huang, Jiangbin Xia

College of Chemistry and Molecular Science, Wuhan University, Wuhan 430072, China

Corresponding author. E-mail: jbxia@whu.edu.cn

Tel & Fax: 86-27-67856707

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1. ¹H-NMR and ¹³C-NMR spectra of the compounds

Figure S1. ¹H NMR (CDCl₃) spectrum of I₂-Pr-EDOT

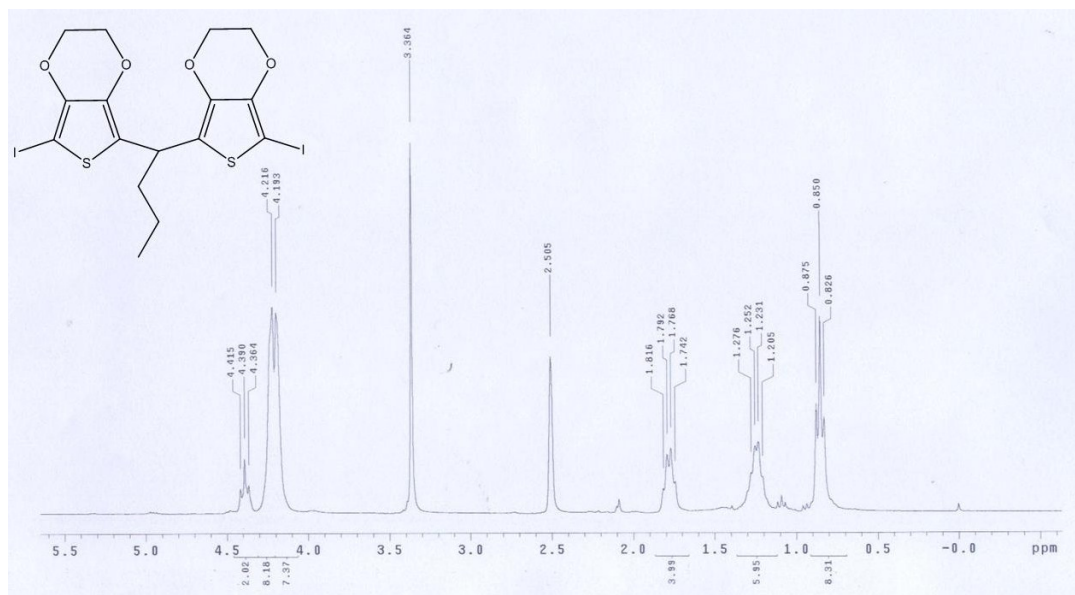


Figure S2. ¹³C NMR (CDCl₃) spectrum of I₂-Pr-EDOT

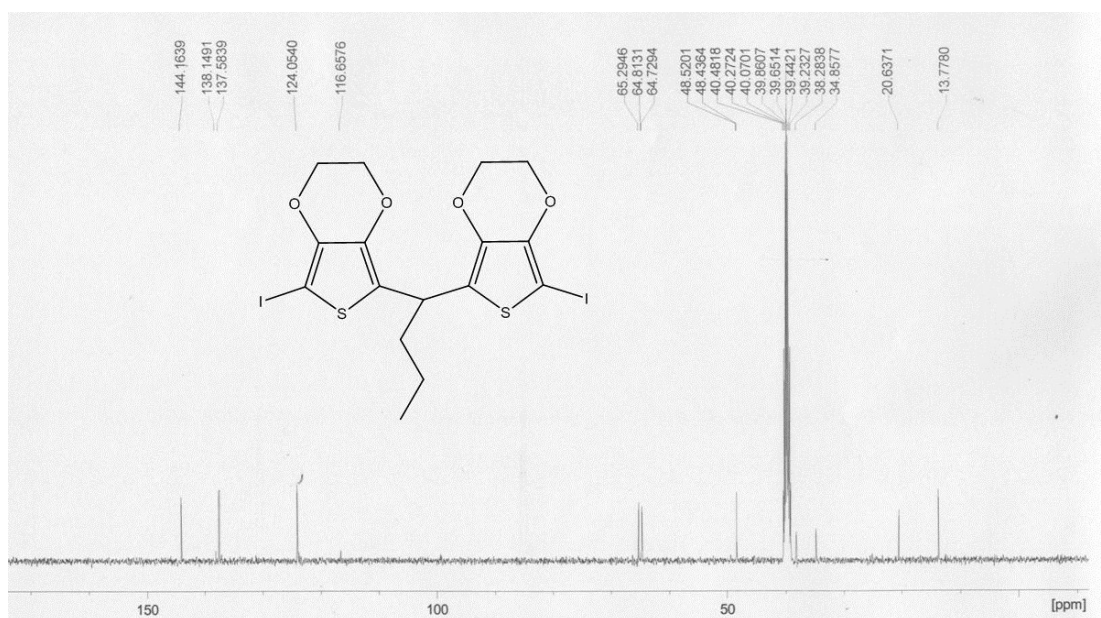


Figure S3. ^1H NMR (CDCl_3) spectrum of $\text{I}_2\text{-Ph-EDOT}$

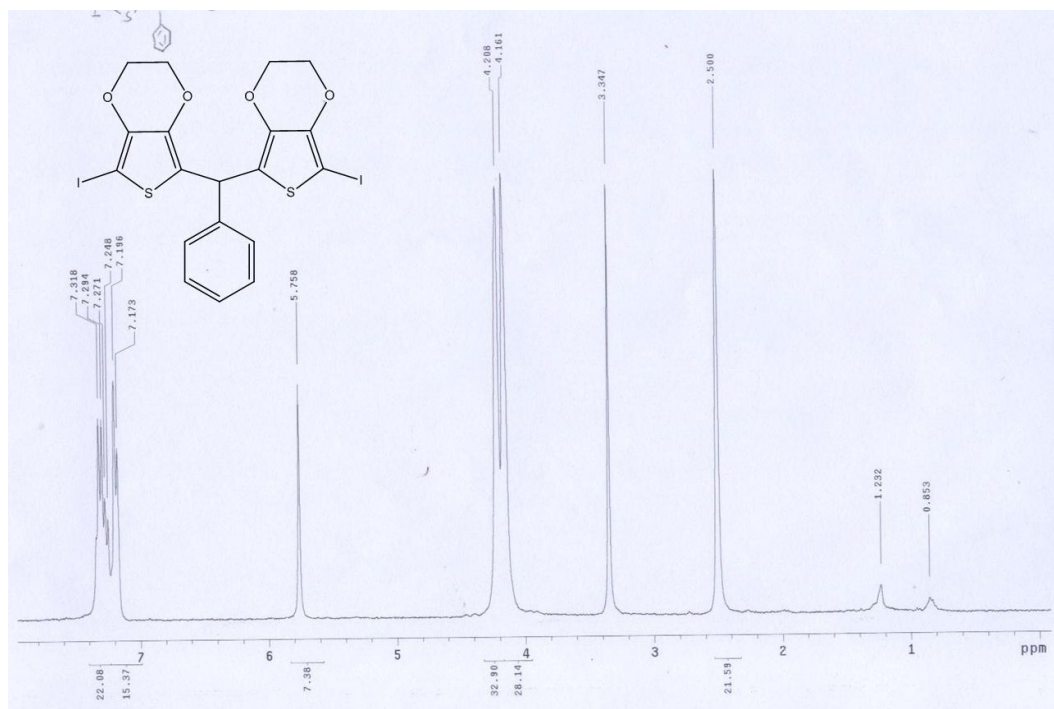


Figure S4. ^{13}C NMR (CDCl_3) spectrum of $\text{I}_2\text{-Ph-EDOT}$

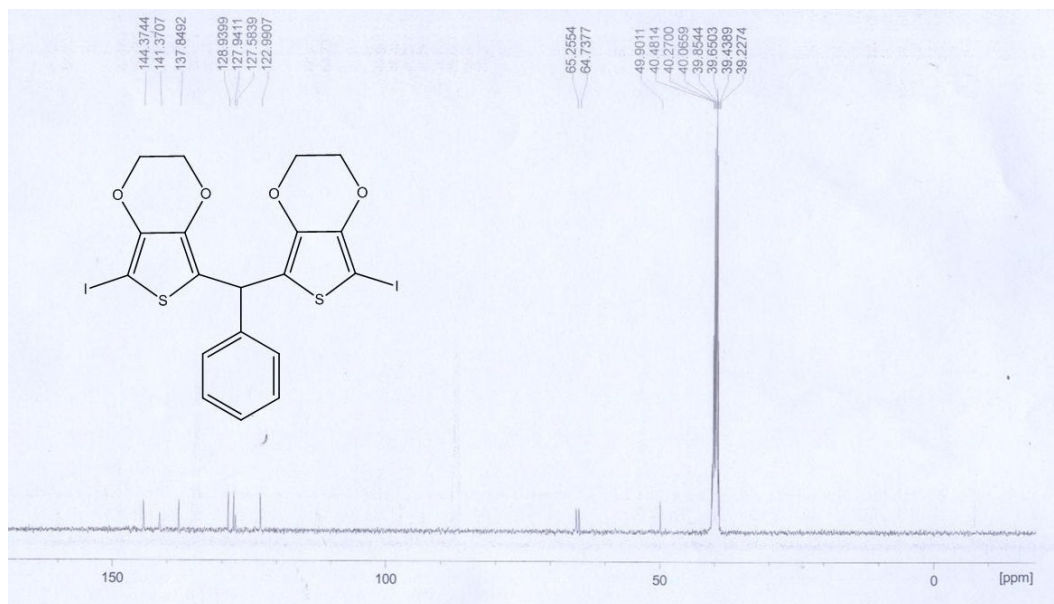


Figure S5. ^1H NMR (CDCl_3) spectrum of $\text{I}_2\text{-Naph-EDOT}$

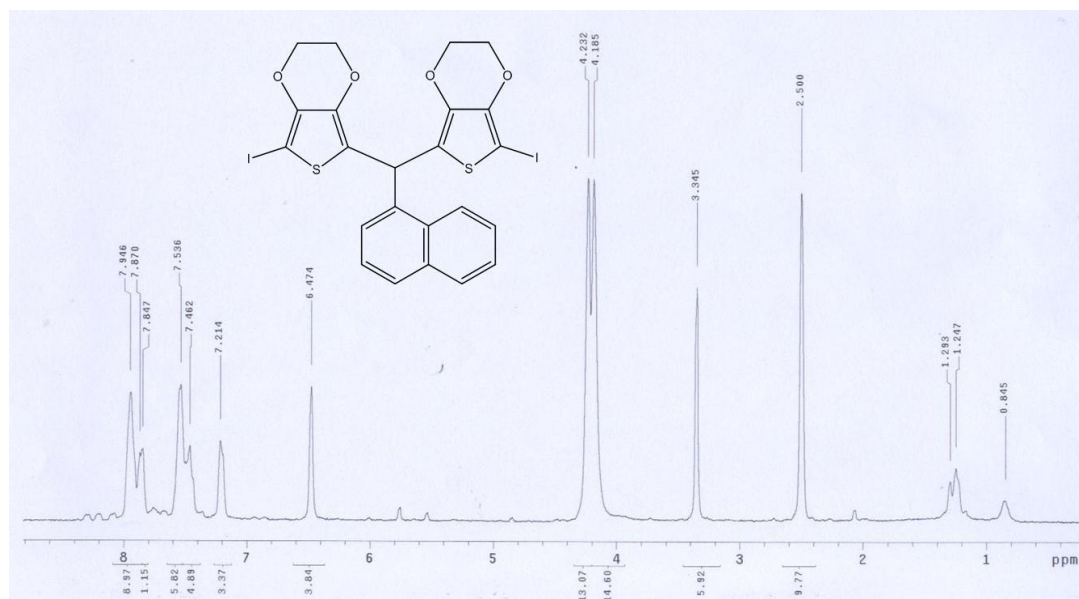


Figure S6. ^{13}C NMR (CDCl_3) $\text{I}_2\text{-Naph-EDOT}$



Figure S7. ^1H NMR (CDCl_3) spectrum of I_2 -Triph-EDOT

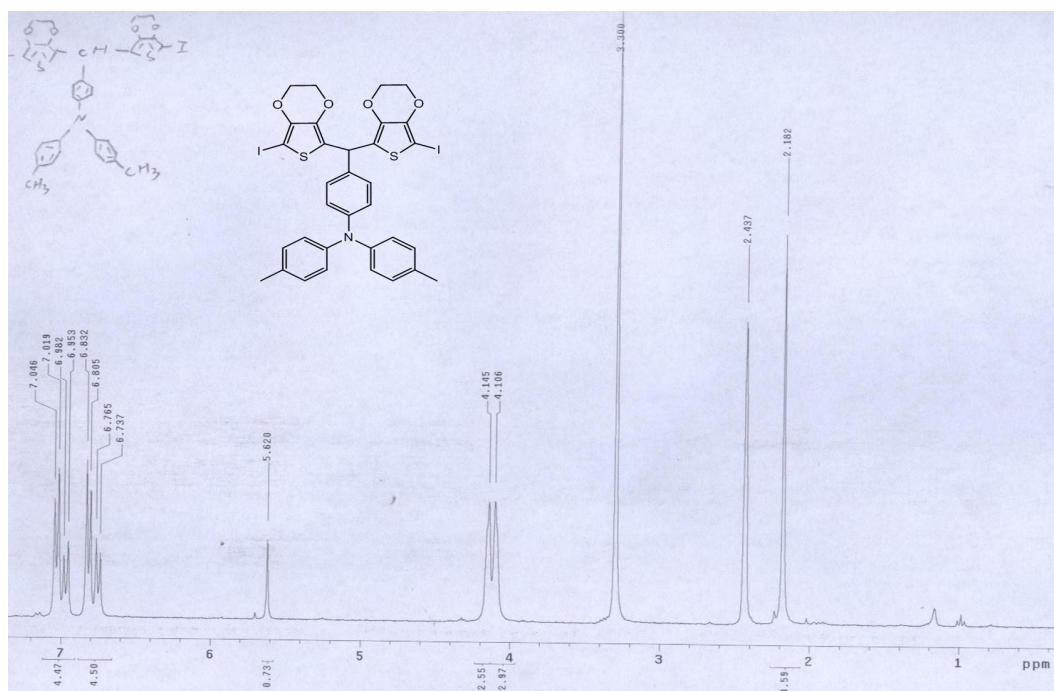


Figure S8. ^{13}C NMR (CDCl_3) spectrum of I_2 -Triph-EDOT

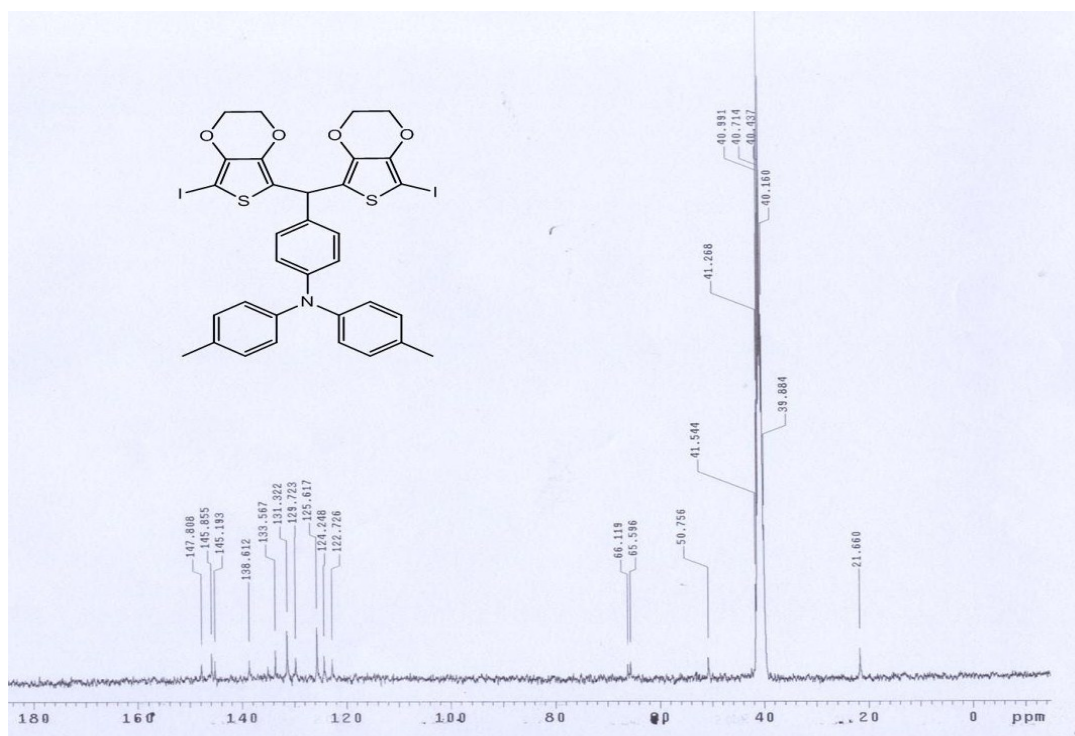
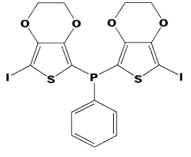
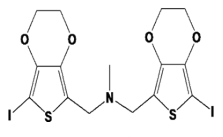
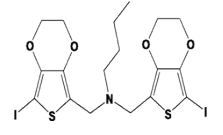
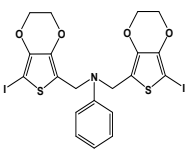
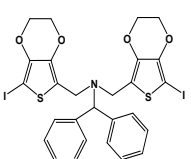
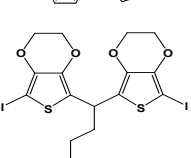
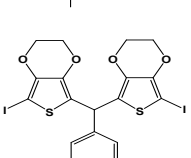
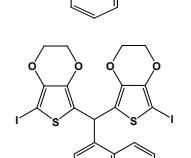


Table S1 Details of the Data Collection and Structure Refinements for All Complexes Reported in This Work

parameter	I ₂ -Ph-EDOT	I ₂ -Nap-EDOT	I ₂ -Pr-EDOT
empirical formula	C ₁₉ H ₁₄ I ₂ O ₄ S ₂	C ₂₃ H ₁₆ I ₂ O ₄ S ₂	C ₁₆ H ₁₆ I ₂ O ₄ S ₂
fw	624.22	674.28	590.21
cryst syst	Orthorhombic	Monoclinic	Monoclinic
space group	P 2 ₁ 2 ₁ 2 ₁	P 21/c	P2(1)/c
a (Å)	16.0830(7)	16.947(2)	8.5162(5)
b (Å)	16.083	9.1615(13)	7.9870(5)
c (Å)	7.8168(4)	15.240(2)	27.2258(15)
α (deg)	90.00	90.00	90.00
β (deg)	90.00	106.051(4)	93.3900(10)
γ (deg)	90.00	90.00	90.00
V (Å ³)	2021.92(14)	2273.9(5)	1848.63(19)
Z	4	4	4
D _{calcd} (g/cm ³)	2.051	1.970	2.121
cryst size (mm ³)	0.2×0.15×0.10	0.2×0.10×0.10	0.12×0.10×0.10
diffractometer	Bruker APEX-II CCD	Bruker APEX-II CCD	Bruker APEX- II CCD
F(000)	1192	1296	1128.0
T (K)	293(2)	293(2)	100(2)
θ _{max}	25.990	28.350	29.99
reflns collected	2340	5642	5351
indep reflns	2304	3338	4991
param refined	244	280	218
R ₁ , wR ₂	0.0184, 0.0440	0.0735, 0.2114	0.0264, 0.1031
GOF (F2)	1.050	1.063	1.255

3. Table S2. T_{onset} of SSP and I/I Distance derived from those monomers (Å)

monomers	effective I/I distance	shortest I/I distance	T_{onset}	Reference
	4.527	4.092	80	1
	4.805	4.131	95	2
	5.479	4.134	80	2
	4.308	4.308	75	3
	4.242	4.055	85	3
	4.878	4.267	70	This work
	4.374	4.374	85	This work
	5.375	5.242	110	This work

1. C. Tusy, L. Huang, K. Peng and J. Xia, *RSC Adv.*, 2014, **4**, 29032

2. C. Tusy, L. Huang, K. Peng and J. Xia *RSC Adv.*, 2015, **5**, 16292.

3. L. Huang, K. Peng, Tong Pei, and J. Xia *RSC Adv.*, 2015, **5**, 70417.