polymers

MDPI

Supplementary Materials

Influence of the Active Layer Structure on the Photovoltaic Performance of Water-Soluble Polythiophene-Based Solar Cells

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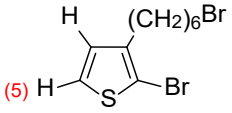
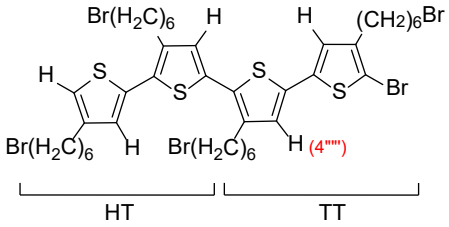
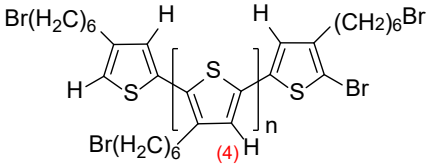
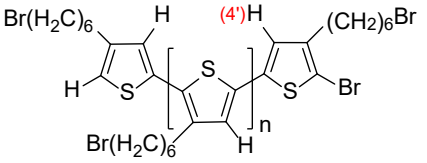
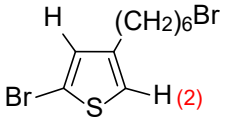
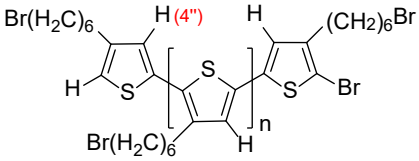
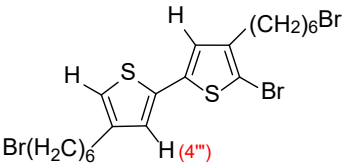
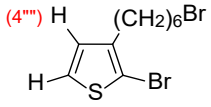
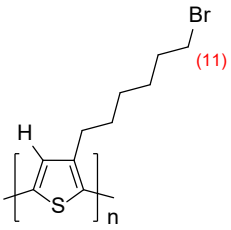
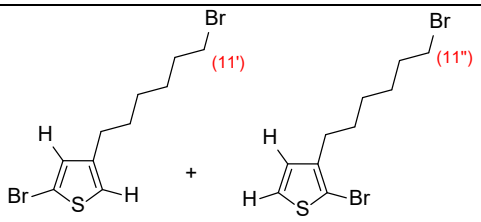
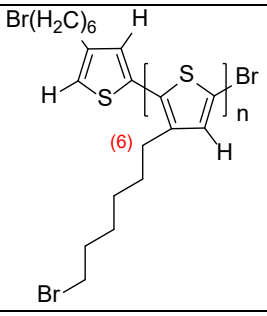
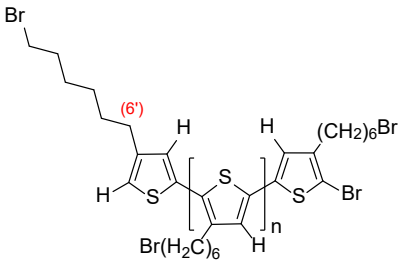
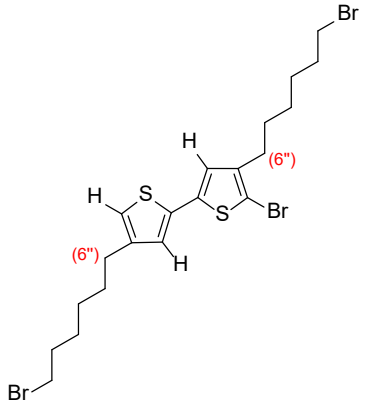
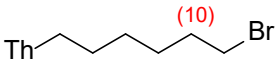
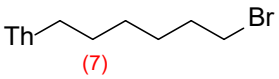
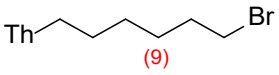
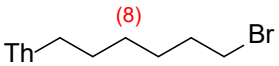
Table S1. Study of PT6Br synthesis by GRIM reaction: chemical shift (ppm) and assignments of the three samples collected at different times.

A (30 min)	*B (60 min)*	*C (90 min)*	*Assignment*	*Ref.*
7.19	7.19	-		[31]
-	7.00	-		
-	6.98	6.98		[32]
-	6.91	-		[33]
6.88	6.88	-		[31]

-	6.87	-		[34]
-	6.81	-		[35,36]
6.79	6.79	-		[31]
-	-	3.43		
3.41	3.41			
-	2.83	2.83		[32]
-	2.65	-		[33,34]

-	2.39	-		
1.86	1.86	1.90		
1.56	1.56, 1.73	1.73		
1.47	1.47	1.49		
1.36	1.36	1.49		

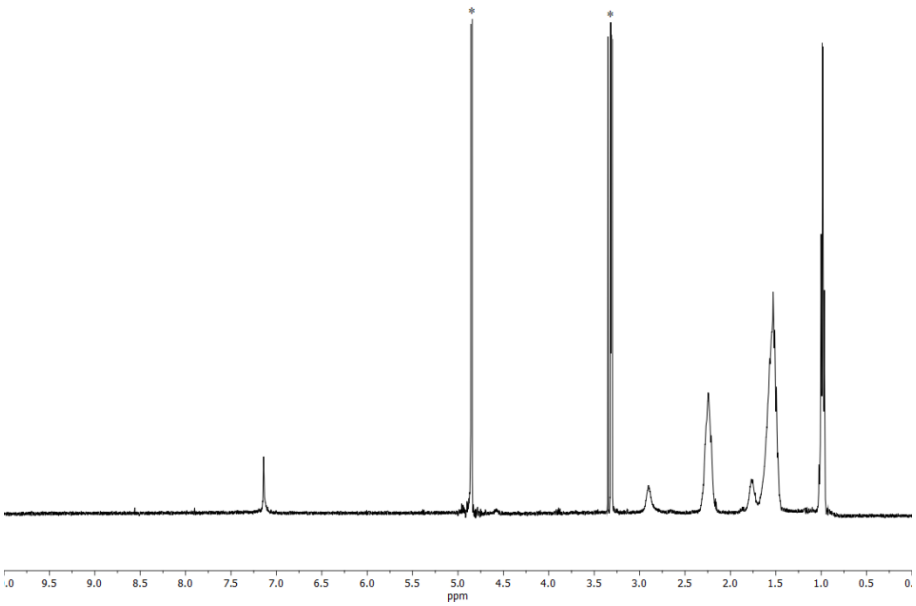


Figure S1. ^{1}H-NMR spectrum of PT6buP^{+}. Asterisk: solvent resonance (CD_3OD).

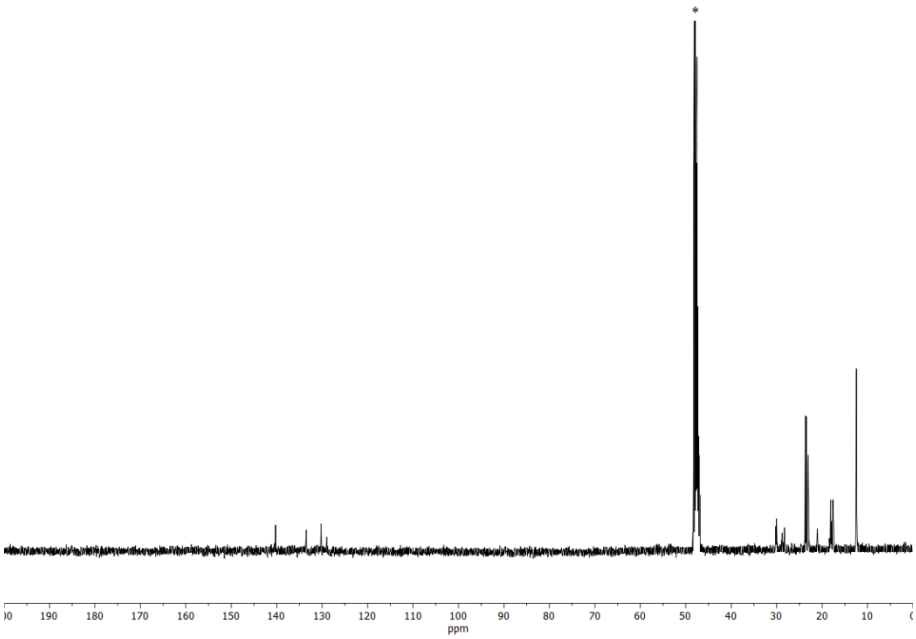


Figure S2. ^{13}C-NMR spectrum of PT6buP^{+}. Asterisk: solvent resonance (CD_3OD).

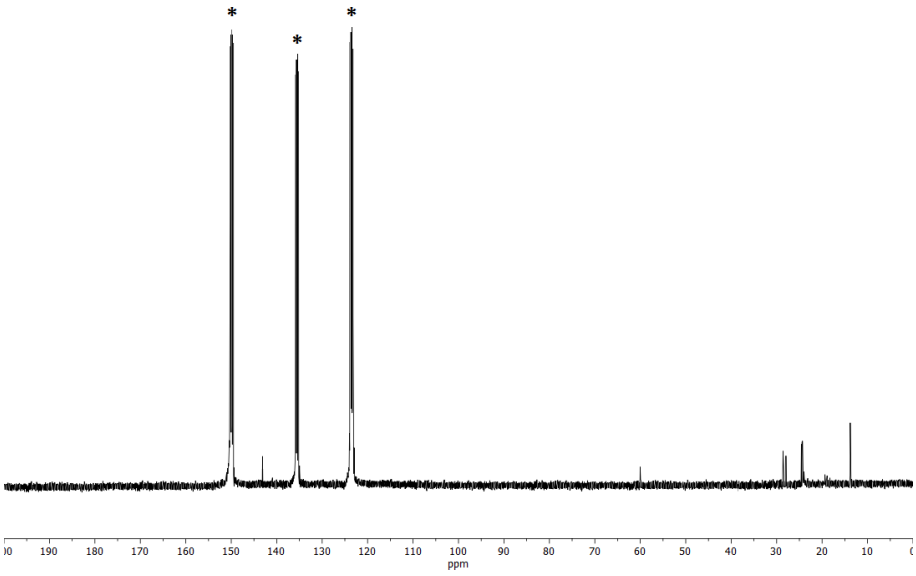


Figure S3. ^{13}C-NMR of P[(T6buP^{+})-*co*-(T6F)]. Asterisk: solvent resonance (pyridine-d_5).

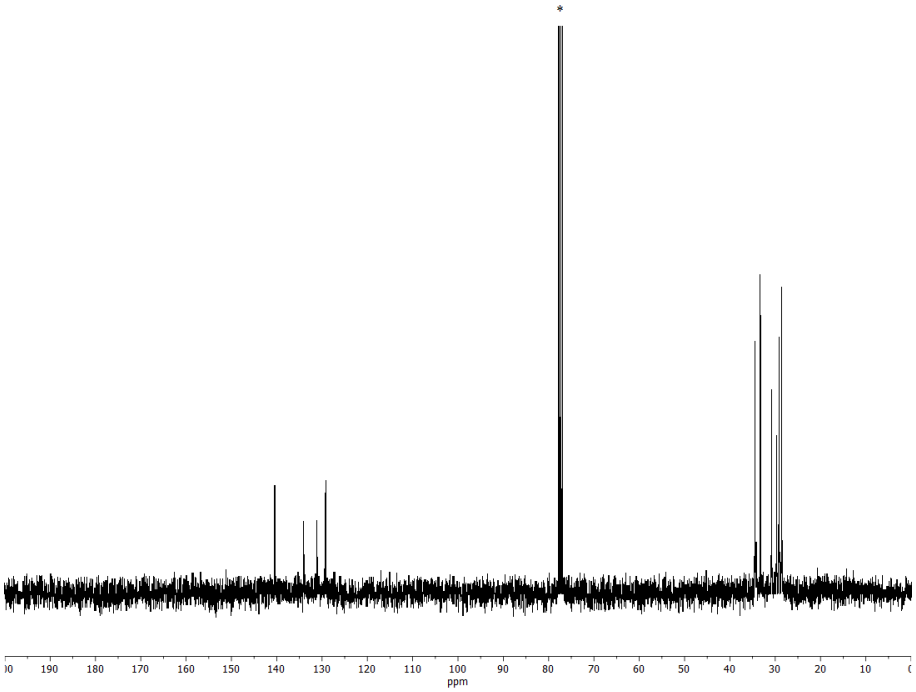


Figure S4. ^{13}C-NMR spectrum of PT6Br. Asterisk: solvent resonance ($CDCl_3$).

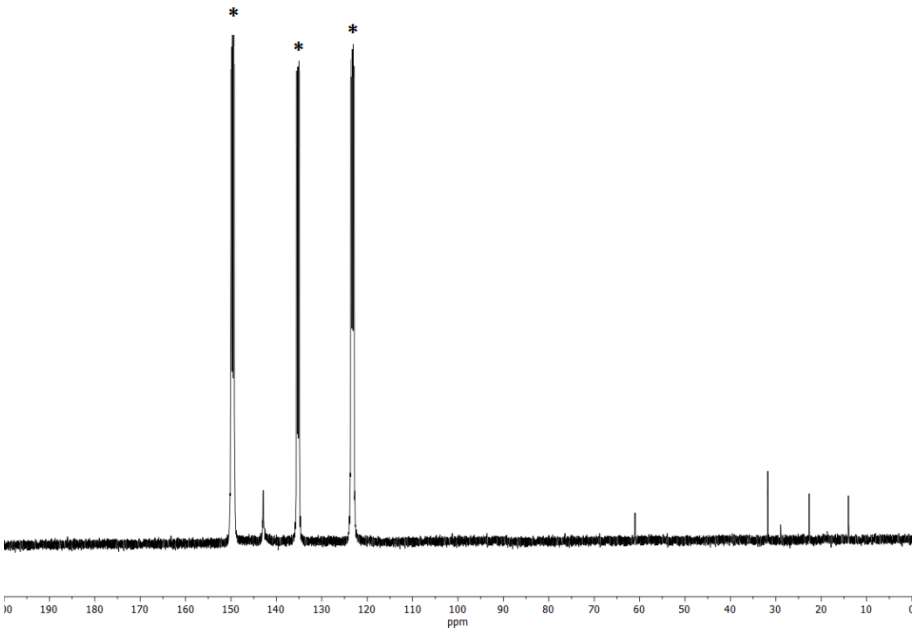


Figure S5. ^{13}C-NMR spectrum of P[(T6Br)-*co*-(T6F)]. Asterisk: solvent resonance (pyridine-d_5).

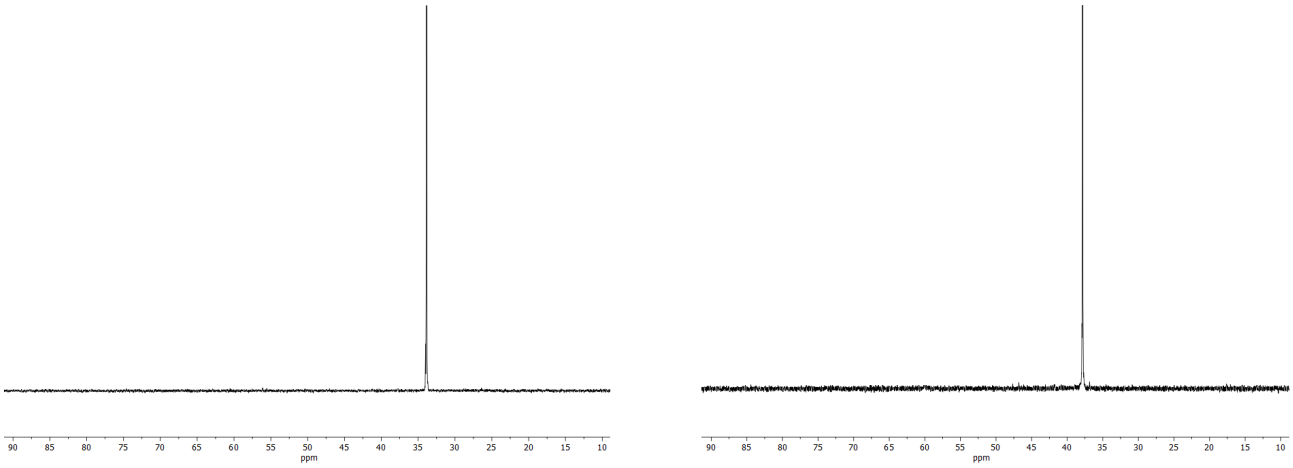


Figure S6. ^{31}P-NMR spectra of PT6buP^{+} (left) and P[(T6buP^{+})-*co*-(T6F)] (right) recorded in CD_3OD.

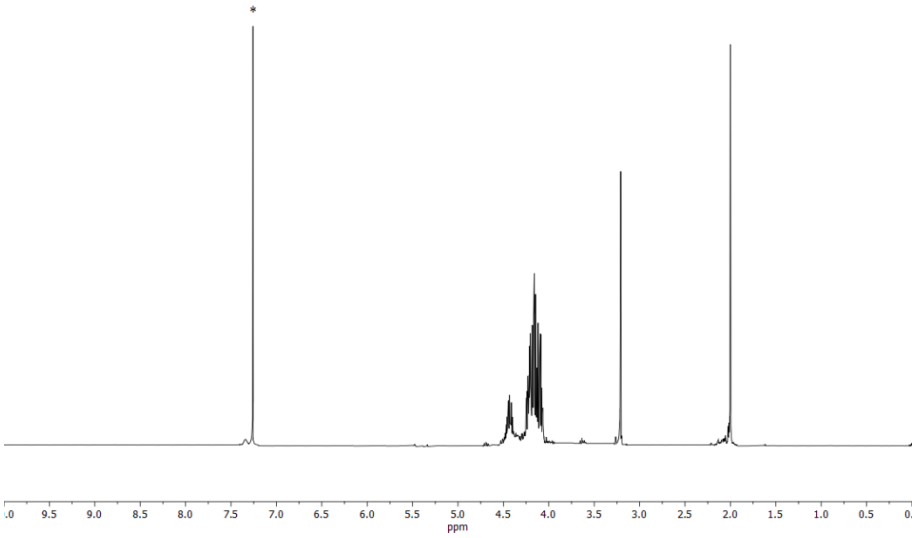


Figure S7. ^{1}H-NMR spectrum of P-Ser. Asterisk: solvent resonance ($CDCl_3$).

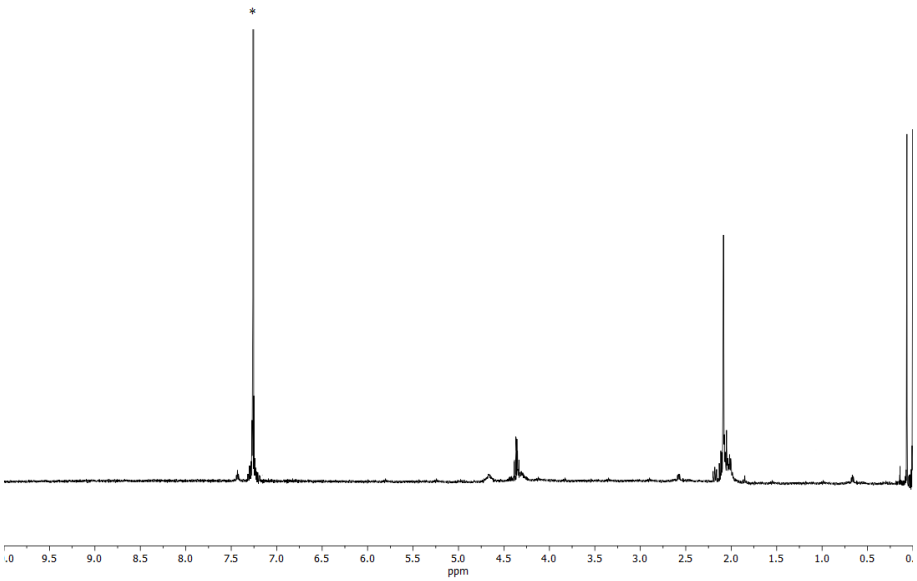


Figure S8. ^{1}H-NMR spectrum of PC_{60}-Ser. Asterisk: solvent resonance ($CDCl_3$).

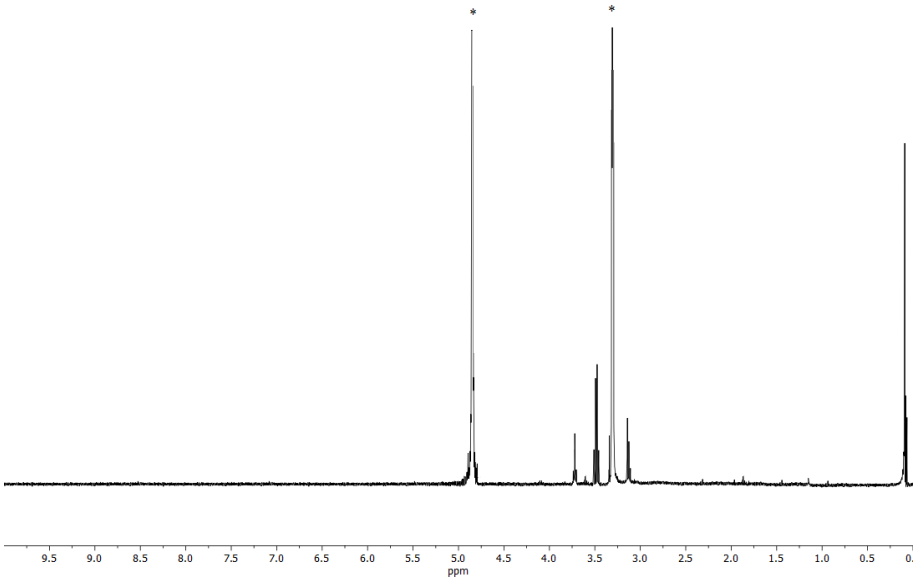


Figure S9. ^{1}H-NMR spectrum of C_{60}-Ser. Asterisk: solvent resonance (CD_3OD).

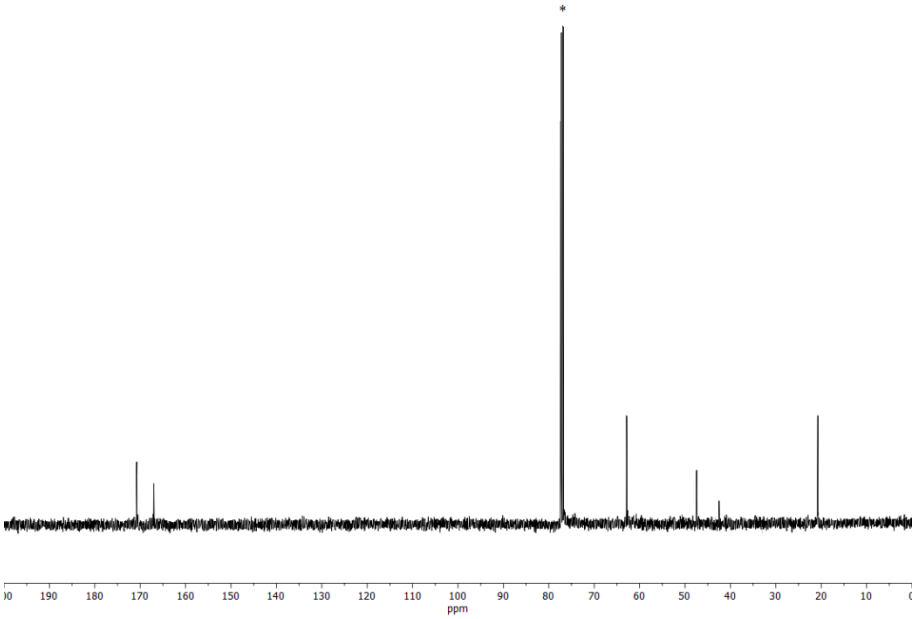


Figure S10. ^{13}C-NMR of P-Ser. Asterisk: solvent resonance ($CDCl_3$).

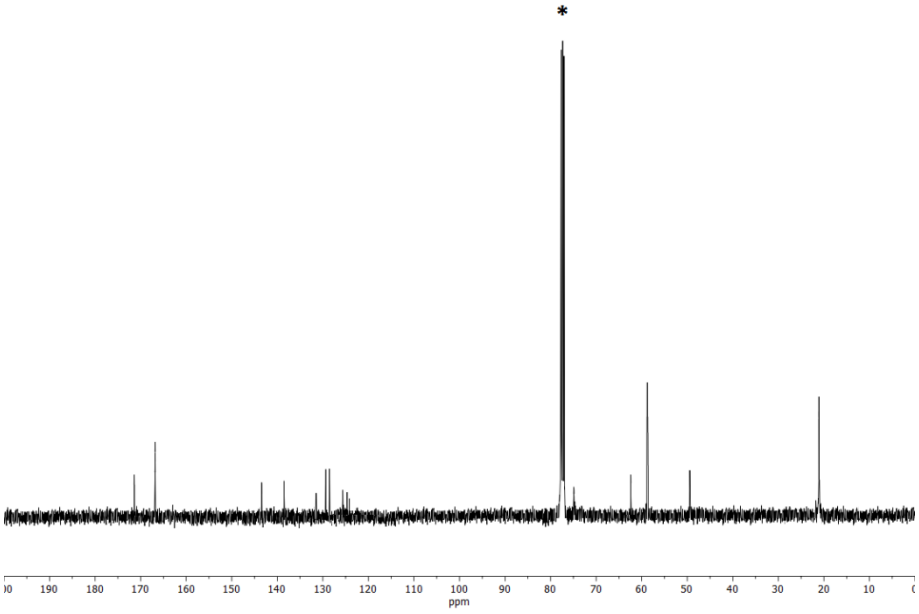


Figure S11. ^{13}C-NMR of PC_{60}-Ser. Asterisk: solvent resonance ().

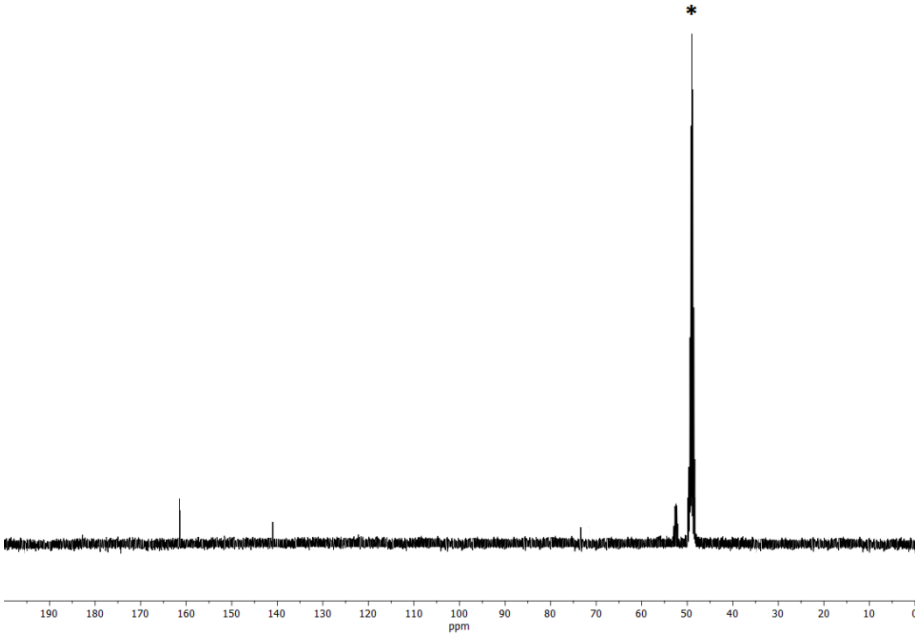


Figure S12. ^{13}C-NMR of C_{60}-Ser. Asterisk: solvent resonance ().

Table S2. Main IR absorption bands (cm^{-1}) of homo-polymers and double-cable copolymers.

PT6Br	***PT6buP$^+$***	***P[(T6Br)-co-(T6F)]***	***P[(T6buP$^+$)-co-(T6F)]***	***Assignment***
3058	3053	3053	3052	υ C-H β thiophene
-	2957	-	2956	υ_{as} –CH_3 (phosphonium group)
2923	2929	2918	2927	υ_{as} -CH_2- (side chain and phosphonium group)
2852	2870	2849	2869	υ_{sym} -CH_2- and –CH_3
1508	1513	1509	1514	υ_{as} -C=C- thiophene
1434	1463	1452	1461	-CH_2- deformation (phosphonium group) and υ_{sym} C=C thiophene
-	-	1428	1427	fullerene
-	1410	-	1408	γ_{as} P-CH_2-R
1384		1384		-CH_3 deformation
-	1378	-	1379	-CH_3 deformation (phosphonium group)
1259	1232	1257	1228	υ C-C thiophene-thiophene
-	-	1181	1180	fullerene
1089	1099	1099	1096	δ –CH thiophene
800	833	826	808	γ C-H thiophene 2, 3, 5-trisubstituted
725	723	722	721	rocking -CH_2-
641, 558	-	644, 557	-	*υ* C-Br aliphatic
-	-	562, 526	576, 526	fullerene

Table S3. Main IR absorption bands (cm^{-1}) of P-Ser, PC_{60}-Ser and C_{60}-Ser.

P-Ser	***PC_{60}-Ser***	***C_{60}-Ser***	***Assignment***
3301	3289	3405	υ N–H
2961	2926	2948	υ_{as} –CH_2–
2902	2853	2623	υ_{sym} –CH_2–
1737	1739	-	υ C=O ester
1661	1646	1649	Amide I band, υ C-O
1537	1543		Amide II band, δ N-H
-	1428	1429	fullerene
-	-	1401	γ OH
1370	1366	1371	Amide III band, υ C-N
1242	1228	-	υ_{as} –$OCOCH_3$
-	1180	1182	fullerene
-	561, 526	576, 526	fullerene

υ = stretching; γ = out of plane bending; δ = in-plane bending.

Thermal properties

TGA analyses

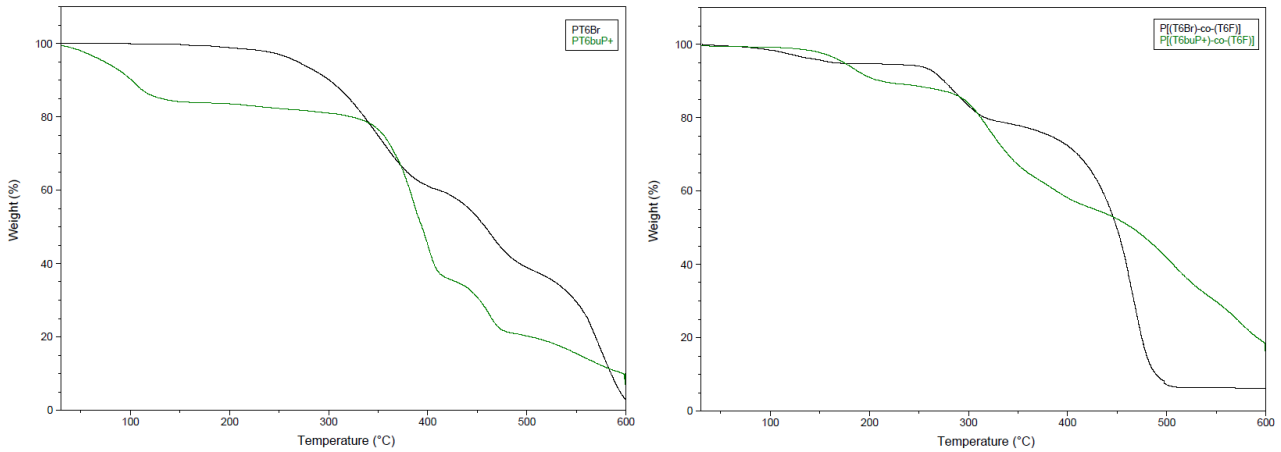


Figure S13. TGA thermograms of homo- (PT6Br and PT6buP⁺, left) and co-polymers (P[(T6Br)-*co*-(T6F)] and P[(T6buP⁺)-*co*-(T6F)], right).

DSC analyses

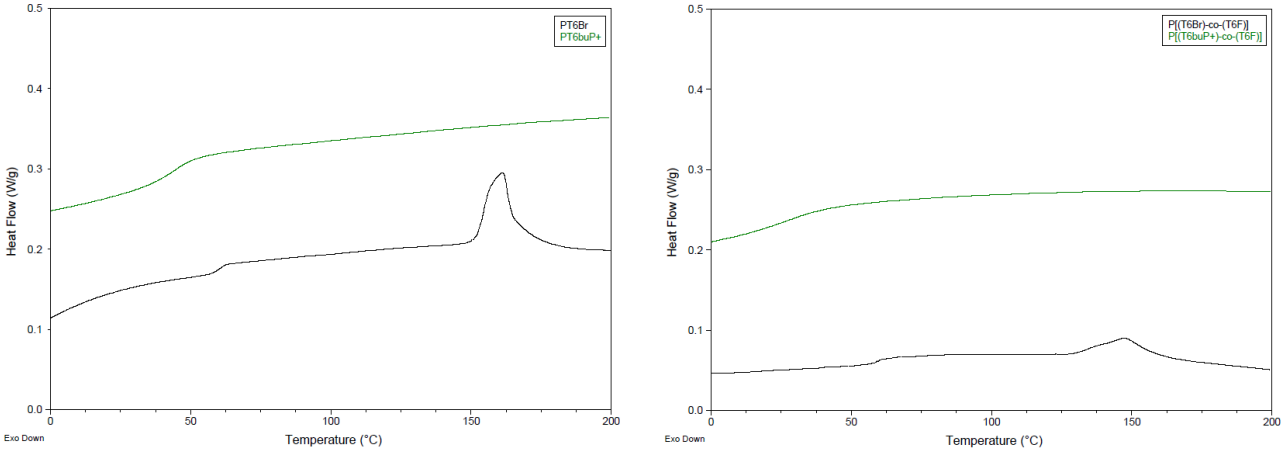


Figure S14. DSC thermograms of homo- (PT6Br and PT6buP⁺, left) and co-polymers (P[(T6Br)-*co*-(T6F)] and P[(T6buP⁺)-*co*-(T6F)], right).