Electronic Supplementary Material (ESI) for RSC Advances

Electronic Supplementary Information for:

Enhanced Absorption Spectra of Conducting Polymers Co-polymerised from Thiophene Derivatives

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Keywords: Conducting Polymers, Polythiophene, Light Absorption, Conjugation, Vapor Phase Polymerization

Absorption coefficients of Th, BTh, TTh and QTh were measured in acetonitrile using quartz cell (figure S1). Experimental data from figure S1 have been used to approximate longer oligothiophenes, due to poor solubility of the material starting from pentathiophene (**figure S2 and S3**). The results show red shift associated with increase in conjugation. Distance between peaks rapidly decreases with increase in conjugation, while intensity of the peak rapidly increases.

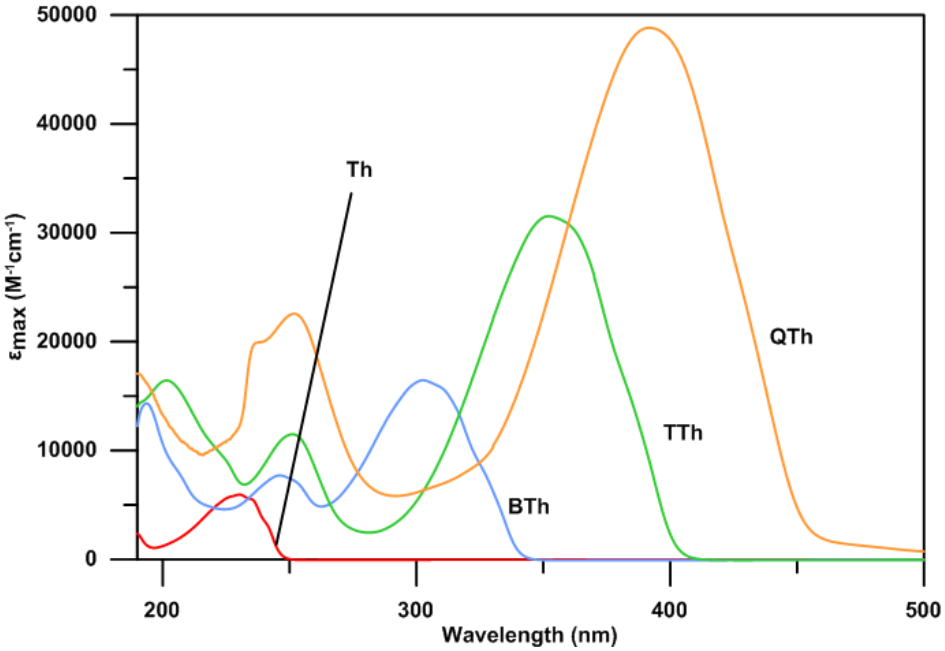

Figure S1 Absorptivity of thiophene, bithiophene, terthiophene, quaterthiophene in acetonitrile.

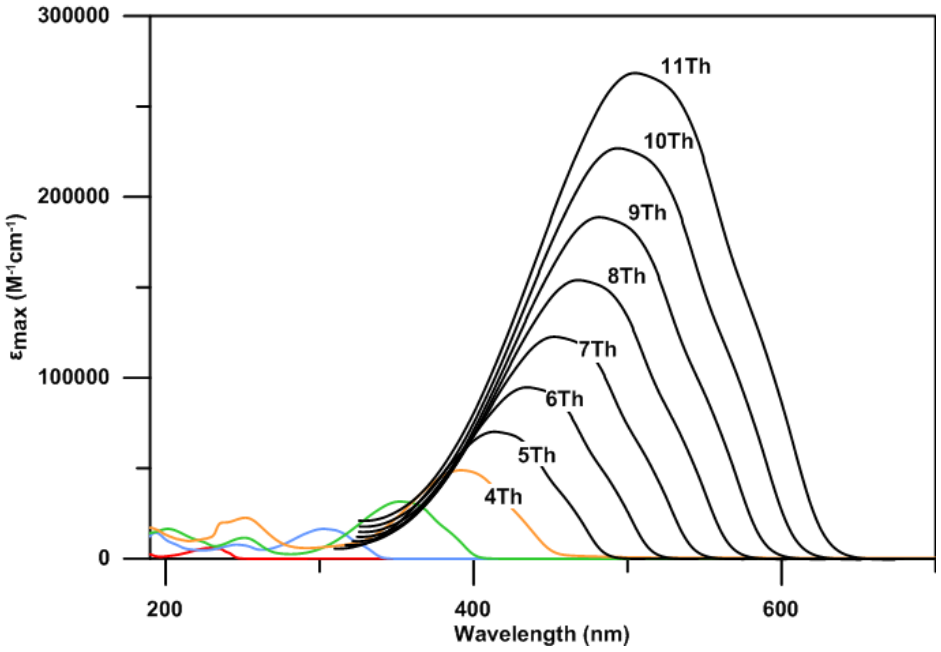

Figure S2 Absorptivity of thiophene, bithiophene, terthiophene, quaterthiophene in acetonitrile and approximated absorptivity of thiophenes from 5Th to 11Th.

Conjugation of poly(bithiophene) corresponds more or less to the predicted conjugation of 11 conjugated thiophene rings, while conjugation of poly(terthiophene) is equal to 9 conjugated rings. Since measurements were taken in acetonitrile, due to difficulty to produce consistent bithiophene, terthiophene and quaterthiophene crystals on glass slide. This study can be used only for estimation of conjugation length. Conjugation of poly(bithiophene) corresponds to 11Th, which is impossible to achieve having only BTh as polymer precursor.

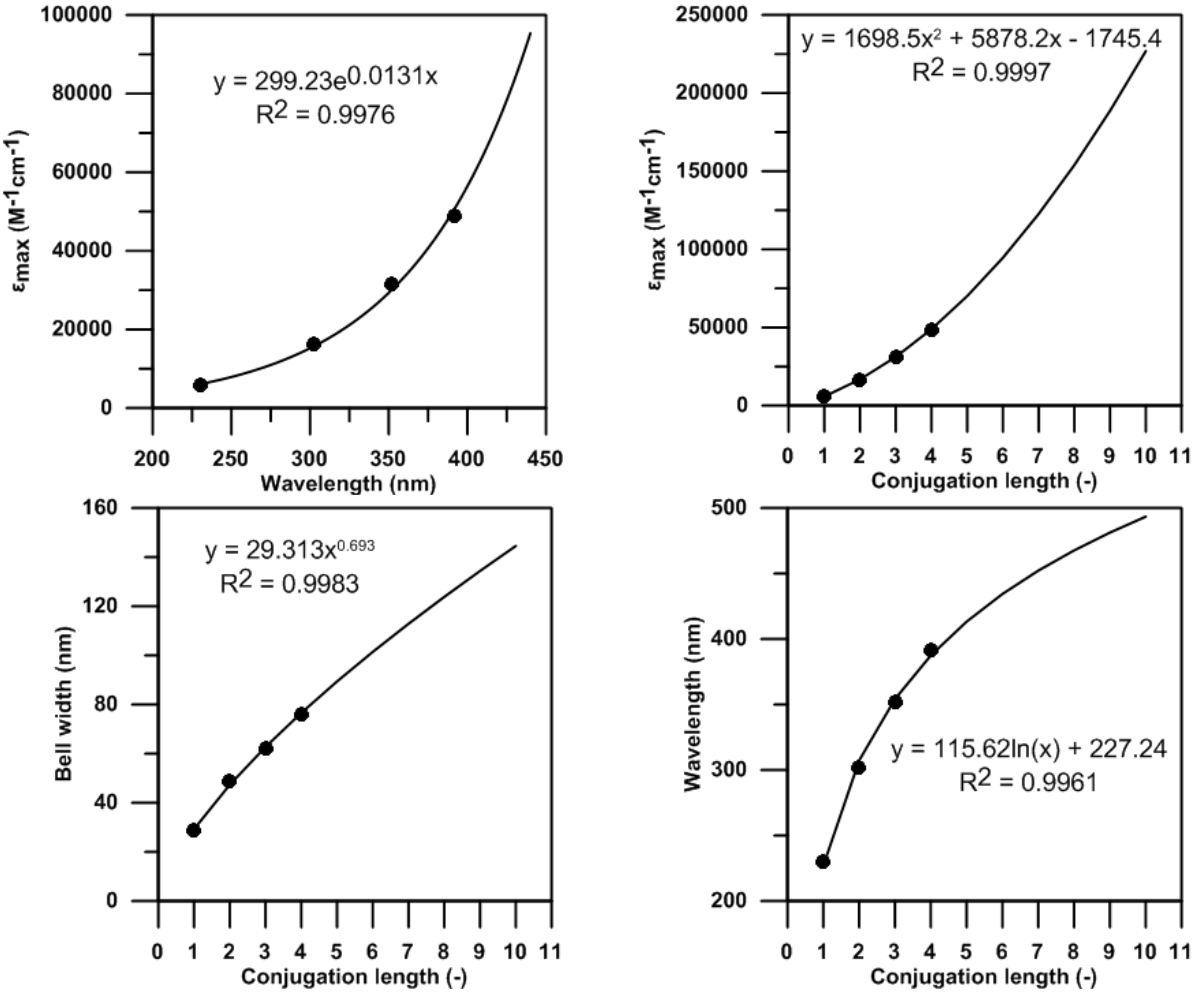

Figure S3 Experimental data gathered from thiophenes and trendline, as an attempt to model longer thiophenes. Relation of absorbivity to peak position (top left), relation of absorbivity to conjugation length of the polymer (top right), relation of peak bell width to conjugation length (bottom left) and relation of peak position to conjugation length (bottom right).

Figure S4 has been plotted based on values calculated using parameters from Table S1. Vapor pressure for terthiophene is very low comparing to vapor pressure of bithiophene. However, both monomers are being used to produce thin film.

Table S1 Vapor pressure parameters for bithipophene and terthiophene.

	2,2'-bithiophene[1]	**2,2':5',2''-terthiophene**[2]
a	35.73 ± 0.18	36.6 ± 0.12
b (K)]	10348 ± 50	13527 ± 42
T (K)	283.14	351.01
p (Pa)	0.442	0.1438
ΔH(kJ·mol^{-1})	86 ± 0.4	112.5 ± 0.3

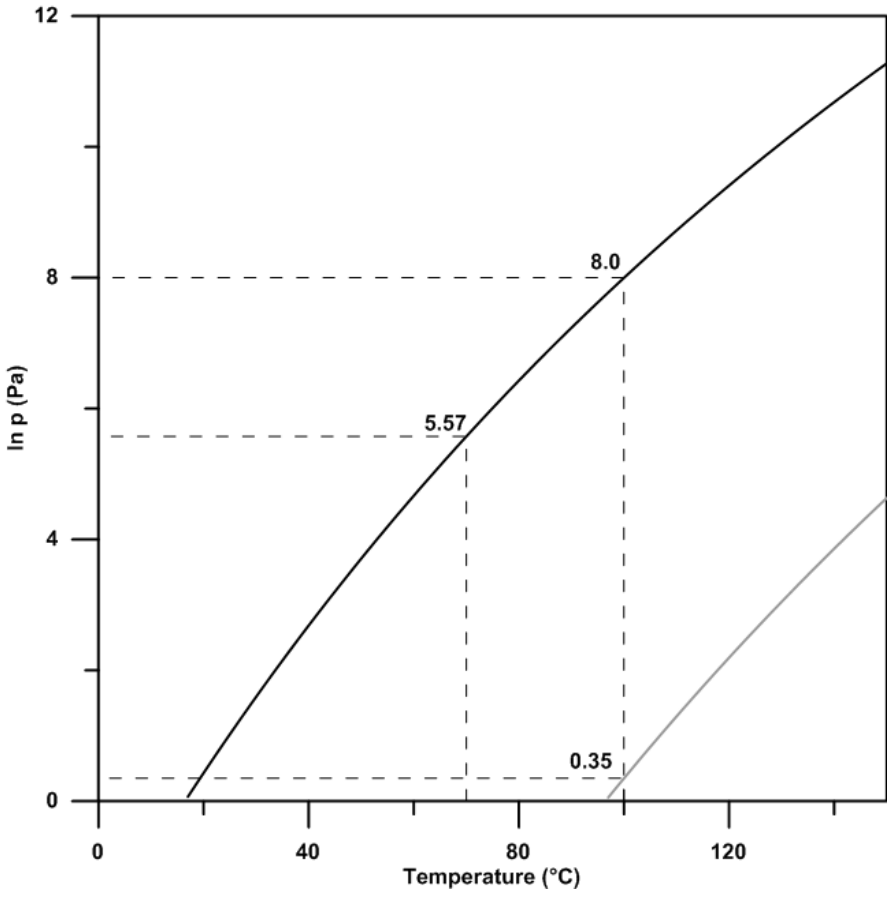

Figure S4 Vapor pressures for bithipophene (black line) and terthiophene (grey line).

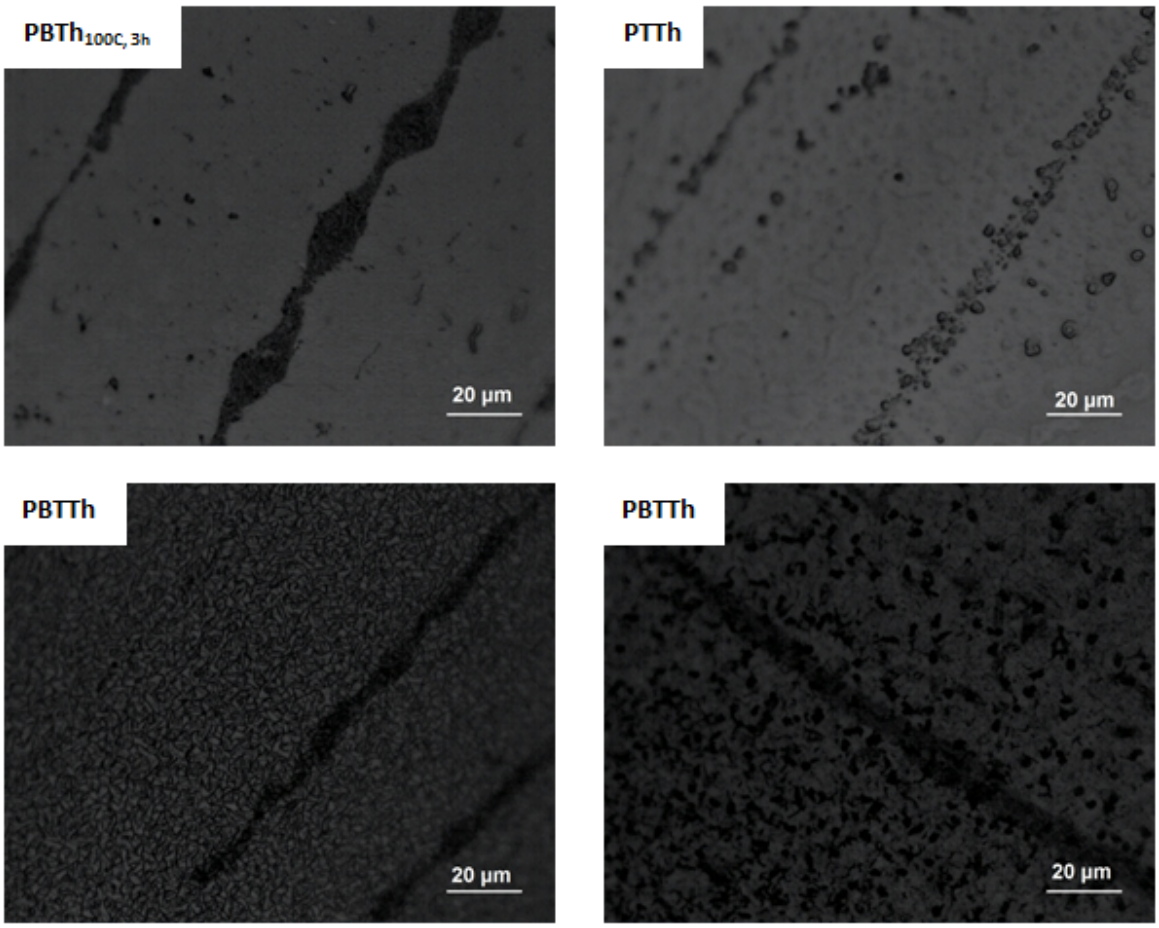

Figure S5 Microscope images of film surface.

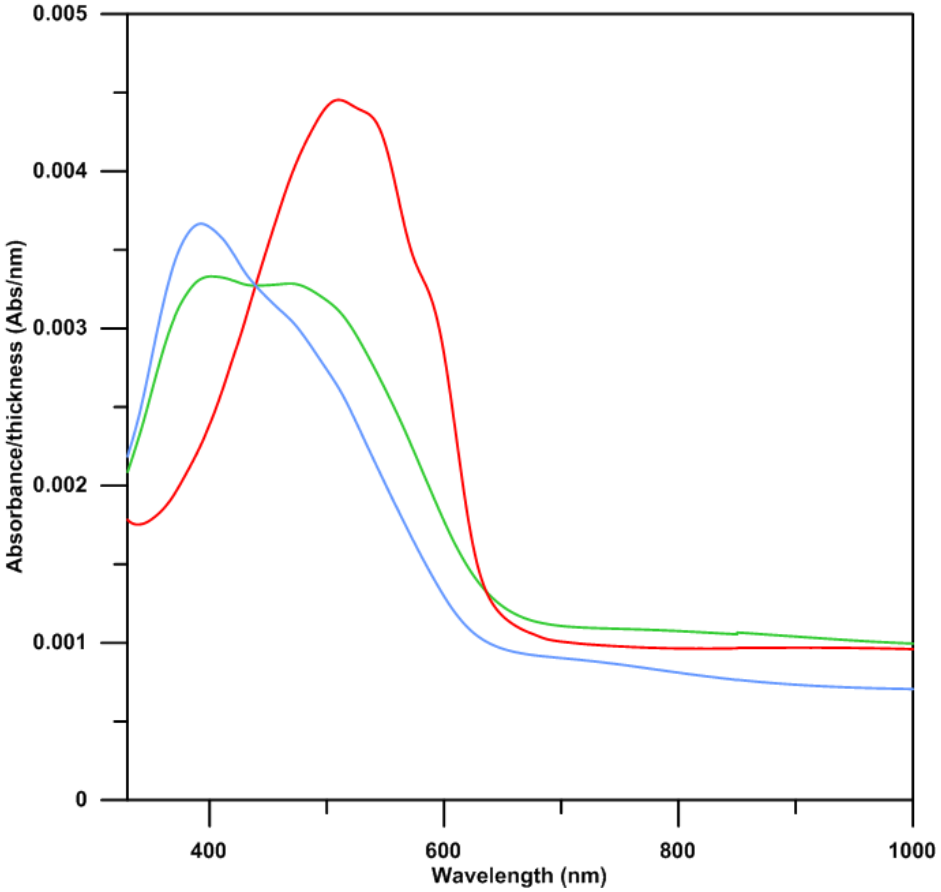

Figure S6 Absorption spectra of (PEDOT:PBTh 1:3):PEG 0.5 (red), (PEDOT:PTTh 1:3):PEG 0.5 (blue) and (PEDOT:PBTTh 1:3):PEG 0.5 (green), normalized to film thickness.

Figure S6 shows blue shift of poly(thiophene) peaks when blended with PEDOT and PEG. This is related to difficulty in penetrating PEDOT:PEG network, especially in case of bigger molecules like terthiophene.

References

1. M. A. V. Ribeiro da Silva, A. F. L. O. M. Santos, J. R. B. Gomes, M. a. V. Roux, M. Temprado, P. Jiménez and R. Notario, *The Journal of Physical Chemistry A*, 2009, **113**, 11042-11050.
2. J. C. S. Costa, C. F. R. A. C. Lima, M. A. A. Rocha, L. R. Gomes and L. M. N. B. F. Santos, *The Journal of Chemical Thermodynamics*, 2011, **43**, 133-139.