Two novel low bandgap, cross-conjugated polymers

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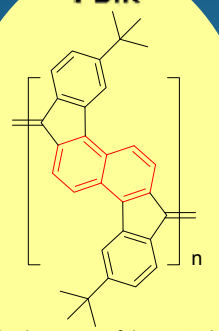
Abstract

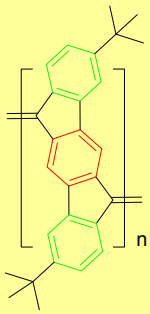
Semiconducting polymers are interesting components for electronic devices e.g. light emitting diodes (OLEDs) or bulk heterojunction-type solar cells. Within this contribution we describe synthesis and characterization of two novel cross-conjugated, aromatic polymers: poly(diindenonaphthalene) **PDIN** and poly(indacenodithiophene) **PIDT**. Within this class of cross-conjugated polymers we have varied the central and the two peripheric aromatic building blocks. **PDIN** with a central naphthalene moiety shows a long wavelength absorption maximum λ_{max} at 727 nm, **PIDT** with two peripheric thiophene moieties a λ_{max} at 644 nm, corresponding to an optical bandgap energy of 1.6 or 1.3 eV, respectively. [1]

PDIN



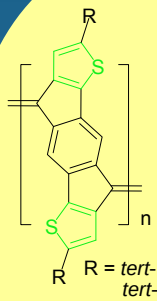
Replacement of the central benzene ring of **PIF** by naphthalene

PIF



Poly(indenofluorene)

PIDT



R = *tert*-Butyl (**a**)
tert-Pentyl (**b**)

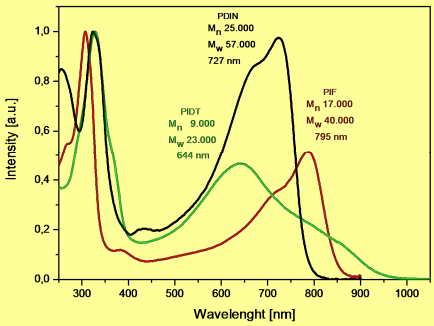
Replacement of the two peripheric benzene rings of **PIF** by thiophene

Experimental Data

Polymer	HOMO	LUMO	bandgap
PIF	5.41 eV[c]	3.95 eV	ca. 1.46 eV
PDIN	5.42 eV[c]	3.84 eV	ca. 1.58 eV
PIDT a)	5.31 eV[d]	4.00 eV	ca. 1.31 eV

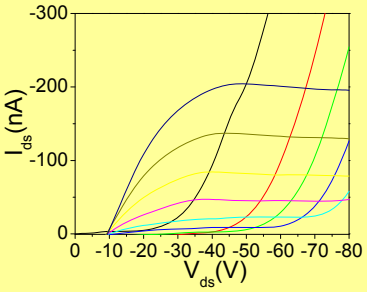
- HOMO level by use of cyclic voltammetry[c] or x-ray photoelectron spectroscopy[d]
- bandgab energy by linear extrapolation of the UV/Vis graph

Optical Properties of PIF, PDIN and PIDT

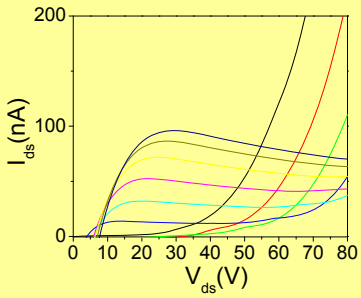


Normalised absorption spectra in CH_2Cl_2

Application of PDIN in Ambipolar OFETs



p-channel



n-channel

Spincoating from o-dichlorobenzene annealing: 150 °C, 10 min

	p-channel mobility (cm^2/Vs)	n-channel mobility (cm^2/Vs)
o-Dichlorobenzene 150 °C	$6x10^{-4}$	$1x10^{-4}$
Chloroform 150 °C	$2x10^{-4}$	$1x10^{-4}$
Chloroform 200 °C	$1x10^{-3}$	$3x10^{-5}$

PDIN: charge carrier mobilities

Conclusion

- Two novel cross-conjugated, aromatic polymers: **PDIN** and **PIDT** have been synthesised and their spectral and photophysical behaviour studied.
- Both polymers show a long wavelength absorption band in the region of 700 - 900 nm being responsible for a small optical bandgap energy.
- The cross-conjugated, aromatic polymers are potential candidates as active semiconducting layers in polymer–based organic solar cells.
- OFET properties of **PDIN** have been studied; measurements to test **PIDT** for OFETs are in progress.
- Future work will be directed to incorporate other building blocks in creating novel cross-conjugated polymers.

References

[1] E. Preis, U. Scherf, *Macromol. Rapid Commun.* **2006**, *27*, 1105-1109.