Organic Semiconductor Materials via Simplified Synthetic Pathways

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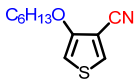
Introduction

In the field of organic semi-conductors (OSC) developed for organic photovoltaic cells (OPV), the environmental impact of the synthesis of organic materials has recently been highlighted.[1] Indeed, the synthetic procedures for the conception of organic semiconductors are essentially based on organometallic couplings or Wittig type reactions giving toxic byproducts. Moreover, the purification of polymers or small molecules often uses large amounts of solvent without ensuring the high level of purity required for semiconductors. The use of direct heteroarylation for the synthesis of conjugated systems is now well established and allows to decrease the environmental impact to do OSCs.[2] In this context, we have focused on the synthesis of new materials for OPV based on the dissymmetric 3-alkoxy-4-cyanothiophene building block[3] by using green procedures. We present here the synthesis of donor – acceptor (D-A) and D-A-D derivatives[4] and the studies of their electronic properties.

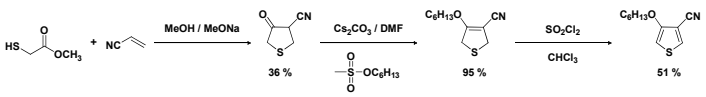
Dissymmetric block



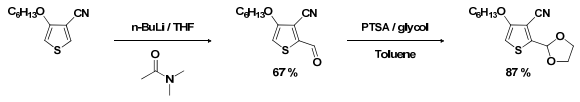
Green Approach for OPV

Synthesis of Precursors

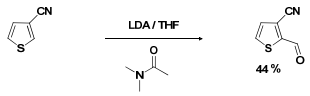
- **Dissymmetric block**



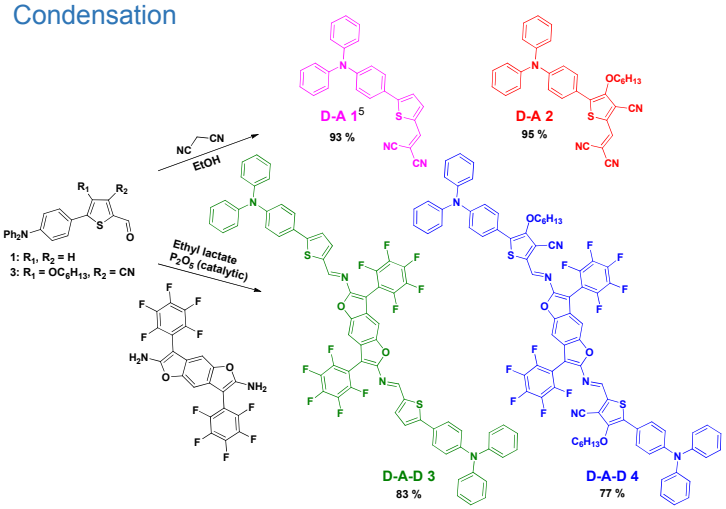
- **Functionalization of Dissymmetric block**



- **Functionalization of 3-cyano-thiophene**

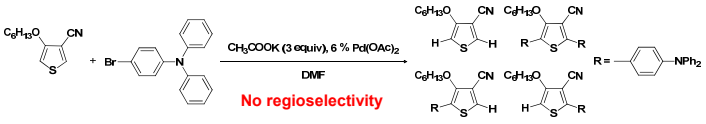


Condensation

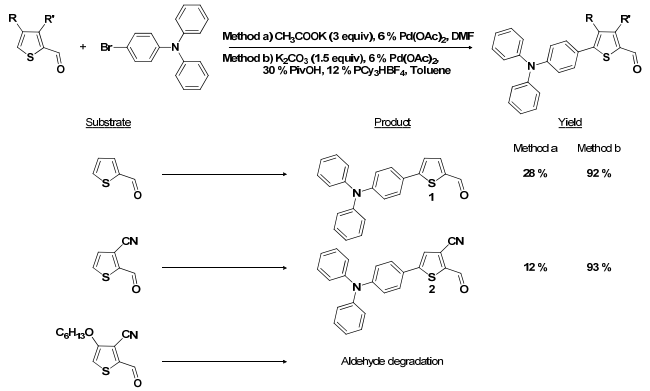


Direct Heteroarylation

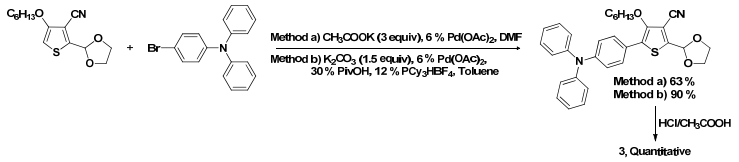
- **Direct Arylation on Dissymmetric block**



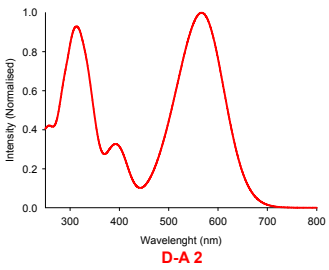
- **Direct Arylation with 4-bromotriphenylamine**

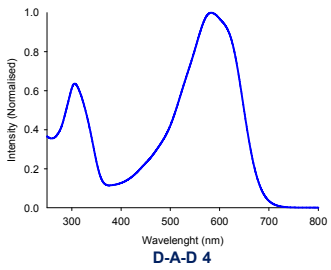


- **Direct Arylation with 4-bromotriphenylamine on Protect Aldehyde**



Optical Spectroscopy





Compound	λ_{max} (nm)	ε ($M^{-1}.cm^{-1}$)	ΔE^{opt} (eV)
D-A 1[5]	501	33900	2.47
D-A 2	567	27 700	2.19
D-A-D 3	536	82 400	2.32
D-A-D 4	582	85 200	2.14

UV – Visible Spectra of compounds **D-A 2** 4.10^{-5} M and **D-A-D 4** 1.10^{-5} M in CH_2Cl_2

Conclusion - Outlook

- We synthesized a new series of D-A and D-A-D materials by following a green approach: direct heteroarylation and condensation.
- The effect of cyano group on building block shows a GAP diminution.
- The optical and electrochemical properties suggest a possible application as donor semiconductors in organic solar cells.

Bibliography

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