

Isoxazole Derivatives With Potential Applications in Polymers and Semiconductors.

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Keywords: liquid crystal, cycloaddition, isoxazole

INTRODUCTION

Organic semiconductors have been receiving significant attention as a new class of electronic materials for organic light emitting diodes (OLEDs), organic field-effect transistors (OFETs), and photovoltaic cells.

The success this technologies in contrast with conventional inorganic semiconductors depends on the way of the deposition of the semiconducting layers, the conjugated π -electron system with high electron affinity, packing geometry; good film-forming properties; chemical stability and purity, etc. These issues are of primary importance in the field of organic electronic materials-OEM.

The purpose of this communication is to show our preliminary results of the synthesis of new liquid crystals through the increase of π -conjugation using the Pd-catalyzed cross-coupling reactions and increase the molecular stability of crystal SmE phase by polymerization or to prepare tripodal molecules.

RESULTS AND DISCUSSION

The isoxazolines and isoxazoles core were synthesized in high yields using the Nitrile oxide [3+2] 1,3 -dipolar cycloaddition of aryl nitrile oxide with 4-X-styrenes as dipolarophiles followed by MnO_2 -oxidation reaction. Using theses reactions we are able to prepare a molecular library including some liquid crystals that have showed SmE mesophase¹. With those molecules in hands, we chose a liquid-crystalline isoxazole and decided to derive it into two different molecular groups:

- To modify the anisotropy of liquid-crystal and extend the π -conjugated system by Sonogashira and Suzuki coupling, comparing the results between them.

- To frozen the SmE crystal properties in the glass state by polymerization of the reactive group at the end of the alkyl chain. And, by reaction with aromatic ring trisubstituted a columnar organization could be envisioned with potential jacketing properties.

Figure 1 describe the potential perspective of 3,5-diarylisoxazoles as intermediate for organic electronic or plastic electronic materials.

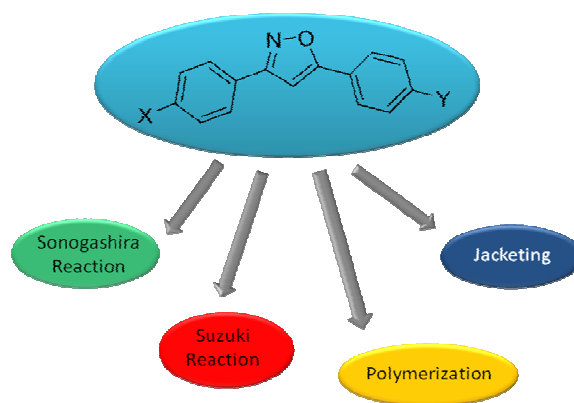
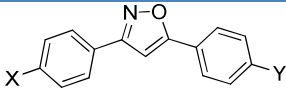
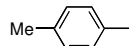
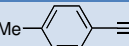
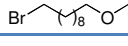


Figure 1. Derivatization of isoxazole into organic and plastic materials.

The data of some intermediates are listed in Table 1. The mesomorphic behavior was analyzed by optical microscopy textures and DSC thermograms.

Table 1. Transitions temperatures for compounds 1-3.

		
X	Y	Transition Temperatures
Me- 	$\text{OC}_{10}\text{H}_{21}$	Cr ₁ 127 Cr ₂ 135 SmC 190 SmA 204 N 254 I
Me- 	$\text{OC}_{10}\text{H}_{21}$	Cr 136 SmC 150 N 251 I
Br- 	Br	Cr 106 SmA 130 I

CONCLUSION

In conclusion, Pd-catalyzed coupling reactions modified the anisotropy and liquid-crystalline behavior of isoxazole. And we synthesized a "jacketing" precursor to synthesize tripodal molecules.

ACKNOWLEDGEMENTS

Support: CNPq; CAPES; INCT-CMN; FAPERGS.

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