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Synthesis of Polythiophenes using Oxidative Coupling

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Using Oxidative Homocoupling

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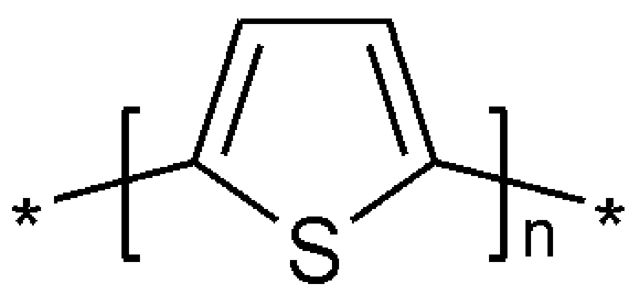
Polythiophenes

Background

Polythiophenes, molecular structure shown below in Figure 1, are polymerization products (also known as polymers) of thiophenes (which are sulfur heterocycles). Polythiophenes become conducting as a result of electron interactions in the conjugated pi-orbitals (of the double bonds) via doping (intentionally adding elemental impurities).This semiconductor-type property of Polythiophenes makes them of special interest to material-science-type applications. They have been dubbed as "synthetic metals".



Recent Studies

The study of Polythiophenes has increased over the last 30 years. The 2000 Nobel Prize in Chemistry was presented to Alan Heeger, Alan MacDiarmid and Hideki Shirakawa for their contribution to the maturation of the field of conducting polymers.

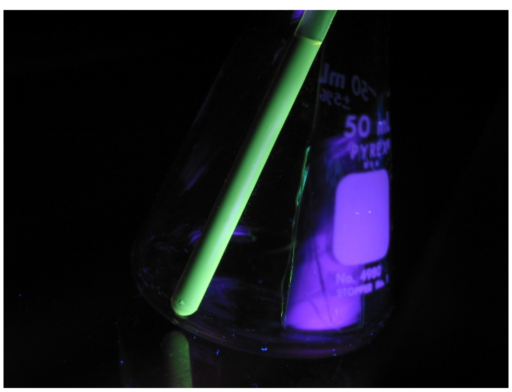
Daily Applications of Polythiophenes

    - Fuel Cells: (doped) Polythiophenes can be used as a conducting polymer in the construction of fuel cells; fuel cells offer us the alternative of a clean energy source
    - Semiconductors in nanotech applications: the conducting nature of conducting polymers make then excellent conducting polymers

- Most common application: Light emitting diodes, (LEDs); the optical properties of Polythiophenes have a huge implementation in the electronic field
- Food chips, sensors: color sensitivity to temperature makes Polythiophenes excellent as indicators of extreme temperature change

Why?

Temperature and doping cause the conjugated back bone of the Polythiophenes to bend which will in turn cause the chemical and physical properties to change. This in the end results in the observed chemical and physical changes in Polythiophenes.



Motivation

Currently existing reactions include the Suzuki Reactions, which produces harmful chemical by products such as borax. The reactions that we are proposing will lead to the production of harmless and chemically benign compounds such as water and hydrogen peroxide.

My Work

The catalysts I was using were sensitive to air. Hence, all reactions had to be done under argon in a glove box. Working with the glove box was not exactly easy, especially using proportions described below:

.02684 gm Benzothiophene
.001347 gm Palladium Catalyst
.1074 Silver Flouride
5 ml DMSO

Where are we in the process?

- Benzofuran to dimer – *success!!*
- Benzothiozole to dimer– *success!!*
- Benzothiophene to dimer – *success!!*
- Other really cool thiophenes from Dr. Lucht's lab to make *poly*mers – experimentation continues!!

All products were analyzed using Gas Chromatography Mass Spectroscopy.

References

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