Cross-Coupling of Regioisomeric Alkylated Benzotriazoles with Thiophene Monomers Yield Conjugated Polymers with Different Optical Properties

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Conducting polymers are a class of organic materials that can conduct electricity. Because of their conducting and semiconducting properties, these polymers are useful as components in solar cells, organic light emitting diodes, transistors and biosensors. These polymers are typically prepared by Stille cross-coupling reactions using stannylated thiophene and bromide monomers. Alkylated benzotriazole bromides are popular building blocks for preparing conjugated polymers due to their electronic properties and solubility-enhancing alkyl groups. Because the triazole group has two possible reaction sites alkylation can give two regioisomers.

Whereas the symmetric 2-isomer has been widely used there have not been reports on the synthesis of polymers with the 1-isomer. This is because the synthesis route of the 2-isomer cannot be used for preparing the 1-isomer. We developed a new synthesis route that allows for synthesizing both the 1- and 2-isomers in high yield. Here we prepared polymers with both the 1- and 2-alkyl benzotriazole isomers by polymerizing with three different stannylated thiophene monomers. The polymers differ in their UV Vis and fluorescence properties showing that the regiosomerism of the alkyl benzotriazole building block affects the optical properties of the polymers.