Synthesis of PCBM Analogues [6,6]-Phenyl-C61-butyric Acid Esters for Efficient Polymer Solar Cells as Electron Acceptors

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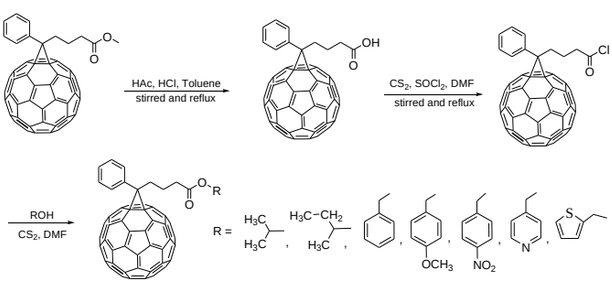
Organic photovoltaics have experienced rapid development and become one of the most vibrant research areas due to their good mechanical flexibility, light-weight, and ease to process.[1,2] Polymer solar cells are one of the most intensively studied OPV systems.[3,4] For polymer solar cells, fullerenes and their derivatives have been recognized as the best acceptor materials due to their unique spherical structures, high electron affinity, and high electron mobility. Soluble fullerene derivatives based on 6,6-phenyl-C61-butyric acid methyl ester (PC61BM) and its C70 analogue PC71BM are the most widely used acceptors for polymer solar cell research.[5,6] A large number of PCBM analogues such as aromatic and heteroaromatic rings, a butyl middle chain, an aliphatic chain, and a methyl end group of ester on PCBM have been studied trying to further improve their properties for polymer solar cells.[7,8] Although remarkable progress has been made, the rules for designing efficient fullerene materials are obscure and rarely discussed, and there is still a lot of space for developing new efficient acceptors through the chemical modification of PCBM. In this work, we synthesized a series of PCBM analogues [6,6]-phenyl-C61-butyric acid ester with alkyl, aryl, thienyl and pyridyl as acceptors through a three-step process involving initial hydrolysis and subsequent acyl chlorination and esterification of PC61BM to systematic research the influence of different ester groups on the polymer solar cells performance (Scheme 1).



Scheme 1 Synthesis of PCBM analogues [6,6]-phenyl-C_{61}-butyric acid esters

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