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Simplified Synthetic Approach to Tetrabrominated Spiro-Cyclopentadithiophene and the Following Derivation to A-D-A Type Acceptor Molecules for Use in Polymer Solar Cells

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Abstract

4,4'-Spiro-bis[cyclopenta[2,1-b;3,4-b']dithiophene] (SCT) is a versatile building block for constructing three-dimensional (3D) π-conjugated molecules for use in organic electronics. In this paper, we report a more convenient synthetic route to SCT and its derivatives, where a structurally symmetric 3,3'-dibromo-5,5'-bis(trimethylsilyl)-2,2'-bithiophene (2) serves as the precursor for both the synthesis of 4H-cyclopenta[2,1-b:3,4-b']dithiophen-4-one (4) and 4-(5,5'-bis(trimethylsilyl)-2,2'-bithiophen-3-yl)-2,6-bis(trimethylsilyl)-4-hydroxy-cyclopenta[2,1-b;3,4-b']dithiophene (5). The later one is the key intermediate for the final brominated SCT building block. Such a "two birds with one stone" strategy simplifies the synthetic approach to the SCT core. Functionalization on the SCT core with different terminal electron-deficient groups, including 1H-indene-1,3(2H)-dione (ID), 2-(3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (IC), and 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (FIC), was carried out, yielding three spiro-conjugated A-D-A type molecules, SCT-(TID)4, SCT-(TIC)4, SCT-(TFIC)4, respectively. The optical spectroscopy and electrochemical properties of these three compounds were investigated and compared to the corresponding linear oligomers. Results revealed that the IC and TFIC terminated compounds showed low-lying HOMO/LUMO energy levels with reduced optical bandgap, making them more suitable for use in polymer solar cells. A power conversion efficiency of 3.73% was achieved for the SCT-(TFIC)4 based cell, demonstrating the application perspective of 3D molecules.

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Biography

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