Title:	Synthesis of Fused Thiophene-based A-D-A Molecules for Efficient Charge Transport and Organic Photovoltaics
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Abstract:	The aim of this work is to synthesize two new acceptor-donor-acceptor (A-D-A) triads for organic photovoltaic applications. The choice of electron donor-acceptor pairs determine the efficiency of charge transport, and hence, the efficiency of the photovoltaic device. The judicious selection of donor and acceptor moieties based on planarity, HOMO/LUMO alignment considerations and density functional theory calculations for geometry optimization is the starting point of the work. The individual donor and acceptor units were successfully synthesized starting from easily accessible benign starting materials and were characterized by 1 H NMR, 13 C NMR, UV/Vis and fluorescence spectroscopy. The synthesis of target ADA molecules have been partially achieved and will be pursued further towards completion. In this work, two A-D-A molecules based on dithienothiophene (DTT) donor and acceptors based on isoindigo and indoloquinoxaline subunits have been designed and partially synthesized. The DTT-based donor was functionalized with acceptors on its either side through through-bond covalent linkage, and the process to purify the final compounds is in progress. After the synthesis, the newly-synthesized molecules will be characterized using 1 H and 13 C NMR spectroscopy, mass spectrometry, UV/Vis absorption spectroscopy, fluorescence spectroscopy, and cyclic voltammetry. Significant effort was also spent in trying to optimize the reaction conditions for the in-house synthesis of DTT starting from thiophene. The results, though not entirely desirable, are promising and encourage further trials to attempt to isolate the pure compound, the synthesis of which presents several challenges. The present study would go beyond this work to explore the charge carrier mobility measurements and photovoltaic device fabrication using a blend of the synthesized molecules as donors and commercial polymer acceptor molecules in a thin film.
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