Low-Temperature Structural Phase Transition in a Soluble Oligoacene and Its Effect on Charge Transport

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— Small-molecule organic semiconductors are of great interest to understanding fundamental properties of charge transport in organic semiconductors as they offer relatively structurally simple model systems. The crystal packing plays a crucial role in determining the electronic performance of a material, as we demonstrate for the case of fluorinated 5,11-bis(triethylsilylethynyl)anthradithiophene. Increased interest in this compound is driven by the recent demonstrations of its high stability and high performance in organic field-effect transistors. This material exhibits a structural phase transition around \( T = 294 \) K, however properties below \( T = 230 \) K have not been investigated in detail. We identify an additional polymorph that forms below \( T = 200 \) K and shows distinct properties compared to the previously reported polymorphs. We identity the phase transition generating the new polymorph using grazing incidence X-Ray diffraction, field-effect transistor electrical characterization and differential scanning calorimetry. The evolution of the field-effect mobility with temperature shows a one order of magnitude increase in value as the films transition from a pure phase to a co-existence of two phases. The structural changes in the film modify the injection picture in these devices, and irreversibly increase the contact resistance two orders of magnitude.