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Quantifying Order in Poly(3-hexylthiophene) CHAD SNYDER, RYAN NIEUWENDAAL, DEAN DELONGCHAMP, National Institute of Standards and Technology (NIST), CHRISTINE LUSCOMBE, PRAKASH SISTA, SHANE BOYD, University of Washington, Seattle — While poly(3-hexylthiophene) (P3HT) is one of the most studied polymers in organic electronics, it remains one of the most challenging in terms of quantitative measures of its order, e.g., crystallinity. To address this challenge, we prepared a series of highly regioregular P3HT fractions ranging from 3.3 kg/mol to 23 kg/mol. Using this series plus a high molar mass (62 kg/mol) commercial material, we compare different metrics for order in P3HT via calorimetry, solid state NMR, and x-ray diffraction. We reconcile the results of our work with those of recent studies on oligomeric (3-hexylthiophenes). One challenge of quantifying low molar mass P3HT samples via DSC is a thermal fractionation effect due to varying chain lengths. We quantify these effects in our molar mass series, and a clear crossover region from extended chain crystals to chain folded crystals is identified through the thermal fractionation process. New values for the enthalpy of fusion of high molar mass P3HT and its equilibrium melting temperature are established through our work. Another result of our research is the validation of high heating rate DSC methods for quantifying crystallinity in P3HT samples with device relevant film thicknesses.

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