Correlating solubility parameters and solvatochromic parameters with the self-assembly of poly(3-hexylthiophene) in mixtures of organic solvents

MADELEINE GORDON, DAVID BOUCHER, College of Charleston — We have studied the assembly and crystallinity of poly(3-hexylthiophene) (P3HT) \((M_n \approx 28.2 \text{ kDa}, \text{regioregularity } > 96\%, \text{PDI } \approx 1.3)\) in >100 binary solvent mixtures using UV-Vis absorption spectroscopy, and it is clear that the identity of the poor solvent used to drive aggregation has a significant impact on the structural order and crystallinity of the P3HT aggregates in solution. Here we report our findings using Hansen solubility parameters (HSPs), specifically the solubility distance vector, \(R_a\), and the Kamlet-Taft solvatochromic parameters of the solvent mixtures to better understand the dominant solvent forces driving the self-assembly of P3HT. We find that the directionality of the \(R_a\) vector provides a better measure of the crystallinity of the P3HT assemblies formed in the solvent mixtures than does the magnitude of the \(R_a\) vector. Our analysis of the Kamlet-Taft (\(\alpha, \beta, \pi^*\)) and \(E_T(30)\) solvatochromic parameters reveals that the \(\beta\) parameter correlates best with the crystallinity of P3HT and that, in general, assemblies having higher structural order are formed in solvent mixtures with lower values of \(\beta\).