

Abstract Submitted  
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**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) ( $M_n \approx 28.2$  kDa, regioregularity  $> 96\%$ , 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  $\beta$ .

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