

Influence of tacticity on solubility of propene monomer in isotactic and syndiotactic polypropylene.

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Abstract

Soly. of propene monomer in isotactic polypropylene (i-PP) and syndiotactic polypropylene (s-PP) is investigated using a Gibbs ensemble Monte Carlo simulation. Tacticity was found to influence the soly., with propene having higher soly. in i-PP. The higher soly. is explained by a more favorable interaction of the propene mols. with i-PP. By analyzing the pair correlation functions of propene with PP it was found that propene favors being in the neighborhood of the PP side Me groups. In addn., it was found that the propene ends orient themselves so that they can be in the proximity of the side methyls. This study provides insight into the effect of tacticity and mol. architecture on soly. in polymers.