Influence of Stereotacticity Defects on the crystallization of Iso-
tactic Polypropylene\textsuperscript{1} XIAOFENG CHEN, RAHMI OZISIK, Rensselaer Poly-
technic Institute, SANAT K. KUMAR, Columbia University, PHILLIP CHOI, Uni-
versity of Alberta, WAYNE L. MATTICE, University of Akron — Monte Carlo simu-
lations of coarse-grained polypropylene on a high coordination lattice were performed 
to investigate the “equilibrium” crystallization behavior of isotactic polypropylene 
with and without stereotacticity defects at various concentrations and distributions. 
The formation of the helical structure, which forms the basic crystalline unit for 
isotactic polypropylene, is the focus of the current study. Results indicate that the 
effect of stereo defects is local - limited to two nearest neighboring repeat units on 
each side of the stereo defect. In addition, the influence of many stereo defects on 
the formation of helices is the sum of the influences of each individual stereo defect. 
The presence of stereo defects retards the crystallization temperature compared to 
isotactic polypropylene with no defects. This is expected as higher undercooling is 
necessary to form helices with imperfections.

\textsuperscript{1}The authors would like to thank National Science Foundation, Procter & Gamble 
Co., and Rensselaer Polytechnic Institute for financial support of this research.