

Abstract Submitted
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Origin of Bends in Unperturbed Vinyl Polymers YERGOU TATEK, WAYNE MATTICE, Institute of Polymer Science, The University of Akron — Sharp bends are observed in highly dendronized polymers when they are placed on a mica surface. One interpretation assumes that thermal fluctuations are responsible for the formation of bends. An alternative explanation would place the emphasis on the stereochemistry of these polymers. We utilized different techniques to find out which one of the above stated explanations is valid. The first approach is based on the average end-to-end vectors calculation of subchains along the polymer backbone, using rotational isomeric states (RIS) model. Bends are located at sites where a drastic variation of these vectors in term of length and direction are observed. A complementary method is to generate, with RIS based Monte Carlo sampling, ensembles of planar conformations, in order to mimic adsorbed polymers on surfaces. By studying these ensembles, one can discriminate bends due to thermal fluctuations from bends due to stereochemistry. Moreover, results for atactic polymers show that stereochemistry is by far the main cause for bend formation. However, RIS based calculations do not take volume exclusion into account. We therefore performed Monte Carlo simulations using bond fluctuation method, of a single chain adsorption. The results appear to be qualitatively similar to the ones obtained with RIS based Monte Carlo sampling.

Yergou Tatek
Institute of Polymer Science, The University of Akron

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