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The Role of Quenched Randomness in the Stereochemical Sequences of Atactic Vinyl Polymers NUMAN WAHEED, WAYNE L. MATTICE, Institute of Polymer Science, University of Akron — The influence of quenched randomness on the mean square unperturbed end-to-end distance, $\langle r^2 \rangle_0$, is assessed in polystyrene, using a rotational isomeric state (RIS) model based on virtual bonds between the centers of mass of the C_6 rings. This coarse-grained model is derived from a conventional RIS model expressed in terms of the C-C bonds in the main chain and contains bond lengths, angles, and torsions determined by the stereochemistry and conformations of the underlying tetrad. The zeroth approximation virtual bond model, which retains only the most probable conformation(s) of the six stereochemically unique tetrads, correctly finds $\langle r^2 \rangle_0 \sim n$in the limit as $n \to \infty$ if the probability for a *meso* diad, p_m, is 0< p_m <1, although the same zeroth approximation model yields $\langle r^2 \rangle_0 \sim n^2$ if p_m is either 0 or 1. The values of $\langle r^2 \rangle_0$ at intermediate p_m are surprisingly close to those obtained from a full, C-C bond based RIS model. This achievement of the zeroth approximation model demonstrates the important role of quenched randomness in determining the unperturbed dimensions of atactic chains. Excellent agreement with the $\langle r^2 \rangle_0$ from the full RIS model over the entire range of stereochemical composition, 0≤ p_m ≤1, can be achieved in a first-approximation virtual bond model, which includes the next most probable conformations at each tetrad and refines slightly some of the conformations by minor adjustments in soft degrees of freedom.

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