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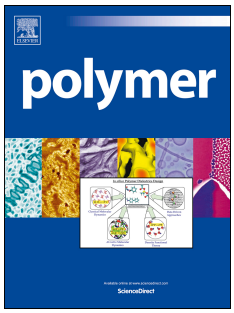

Effect of an asymmetry of branching on structural characteristics of dendrimers revealed by Brownian dynamics simulations

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Effect of an asymmetry of branching on structural characteristics of dendrimers revealed by Brownian dynamics simulations

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Abstract

Dendrimers in dilute solution with asymmetry of branching were simulated by the Brownian dynamics method. In this simulation a coarse-grained dendrimer model and athermal solvent conditions were implemented, extending previous work to a wider range of branch asymmetries at fixed average spacer lengths and high generation numbers close to the theoretical limit. We considered both global and local structural characteristics of dendrimers. The global ones such as, the average distance of ends from the center, the radius of gyration, the hydrodynamic radius and the dendrimer shape anisotropy are practically insensitive to the asymmetry of branching. The effect of the spacer asymmetry is revealed mainly in the local structure of dendrimers. In particular the radial density profile changes its shape from a convex to a concave one with an increase of the asymmetry. As compared to symmetrical case, the distribution of terminal monomer units in asymmetrical dendrimers shifts towards the dendrimers periphery. The terminal monomers in an asymmetrical dendrimer are on average in a denser environment compared to their symmetrical analogs. The shorter spacers are less stretched and more turned back to the core than

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