MOLECULAR DYNAMICS SIMULATION OF DENDRIMERS IN THE LENNARD-JONES SOLVENT

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Series of computer simulation of dendrimers (see [1]) essentially advanced the understanding of spatial structure and molecular mobility of these unusual polymeric structures. However, numerical experiments were generally performed without explicit account of solvent molecules: a solvent influence was simulated by variation of the potential parameters of van der Waals interactions [2,3]. Recently the behaviour of the dendrimer in the explicit solvent has been considered for Meijer dendrimer box [4] and for a crude bead-spring model of dendrimer [5]. In this work, we study the effect of an explicit solvent on the structural and dynamic properties in the framework of a detailed molecular model of two dendrimers of close topology.

Simulations were been carried out for carbosilane and poly(propylene imine) dendrimers of 5th generation under periodic boundary conditions at different temperature. Calculations have been accomplished using the AMBER force field in the united atom approximation. Lennard-Jones particles have been considered as the solvent molecules with potential parameters corresponded to CCl4.

The internal organization of dendrimers was analyzed (gyration radii and principal moments of inertia, density distributions for both dendrimer and solvent atoms) as well as dynamic properties of dendrimers (frequencies of conformational transitions, mobility of different center of branching, rotation and translation diffusions), and mobility of solvent molecules. The results obtained were compared with the data of calculations made with implicit account of the solvent and experimental data.

This work was supported by NWO (project no. 99 005 725) and INTAS (project no. 00-00712).

References

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