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Evaluation of fractal dimension of star polymers with different numbers of arms in computer experiment

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Abstract

One of the important characteristics of a polymer molecule is its fractal dimension. Fractals are objects whose Hausdorff dimension is fractional and exceeds the topological dimension. The main distinguishing feature of such objects is self-similarity. The fractal characteristics of polymer macromolecules largely determine the chemical, physicochemical, and physical properties of these objects, such as the Mark-Kuhn-Houwink scaling parameters, toughness, tangent of the angle of mechanical losses, and dynamic modulus of elasticity. Today the fractal properties of topologically linear polymers are studied in detail, however, the fractal properties of practically significant star polymers are still poorly studied. This is probably due to the fact that computer simulation of polymer systems by methods of classical mechanics requires lengthy calculations even on supercomputers. In this regard, it is interesting to evaluate the possibility of using relatively simple software packages such as HyperChem in molecular modeling of polymers.

The purpose of the research was to determine the fractal dimension for 3, 4, 5, and 6-arm star $(\text{-}CH_2\text{-}CH_2\text{-})_n$ polymers in a state of minimum potential energy in an isolated system and in a state of thermodynamic equilibrium at a constant temperature, comparing the obtained values with the fractal dimension of linear polyethylene and to mfke an assessment of the appropriateness of using the HyperChem software package for macromolecular calculations. A computer experiment was conducted using the HyperChem package. To obtain isolated molecules in a state of minimum potential energy, a simulation by the conjugate gradient method was performed. To bring the macromolecules to a state of thermodynamic equilibrium at a constant temperature, the molecular modeling in the canonical ensemble was carried out. For the studied polymers, the values of the fractal dimension and critical Flory index were calculated. The data obtained confirm the relation between fractal dimension and conformation of the macromolecule and, within the accuracy achieved, indicate the absence of fractal properties for star macromolecules with a large number of arms.

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