Название публикации:
Quantum-Chemical Study of Stressed Polyethylene and Butadiene Rubber Chain Scission

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Аннотация:
The thermal decomposition of polyethylene and butadiene rubber chains in the presence of a tensile force acting along the axis of the molecule was simulated. The reaction of an isolated chain was considered. The chain models were the octane and 2,6-octadiene molecules. A deformation was introduced in the problem by fixing nonequilibrium distances between the terminal carbon atoms. The reaction coordinate (the middle C-C bond length R) was scanned at a fixed length of the molecule (L). That is, the potential energy surface section of the reaction was constructed at L = const. The reaction sensitivity to deformation was evaluated by B3LYP, LC-omega PBE, CCSD(T), CASSCF, and MP2 quantum-chemical calculations. All these calculations showed that the molecule elongated by 1 for polyethylene, but shortened by 0.3-0.5 for 2,6-octadiene during chain scission. This means that the tensile deformation accelerates the decomposition of polyethylene, but decelerates the decomposition of butadiene rubber.

Ключевые слова:
Mechanical activation; methyl radicals; mechanochemistry; abstraction; cyclohexane; kinetics; alkanes; ozone; bonds