Название публикации:

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

Авторы:

Krisyuk, B.E.a, Mamin, E.A.b,c, Popov, A.A.b,c

a. Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Moscow oblast, Russian Federation
b. Plekhanov Russian University of Economics, Moscow, Russian Federation
c. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, Russian Federation

Сведения об издании:

Quality - Access to Success
Volume 19, Issue 164, 1 June 2018, Pages 43-47

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-ωPBE, CCSD(T), CASSCF, and MP2 quantum-chemical calculations. All these calculations showed that the molecule elongated by ~1 Å for polyethylene, but shortened by 0.3–0.5 Å 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:

chain scission reaction, kinetics, mechanical deformation, mechanical stress, quantum chemistry