QUANTUM CHEMICAL STUDY OF REACTION MECHANISM OF 2,3-DIMETHYLBUTA-1,3-DIENE AND METHYL ACRYLATE [4+2]-CYCLOADDITION

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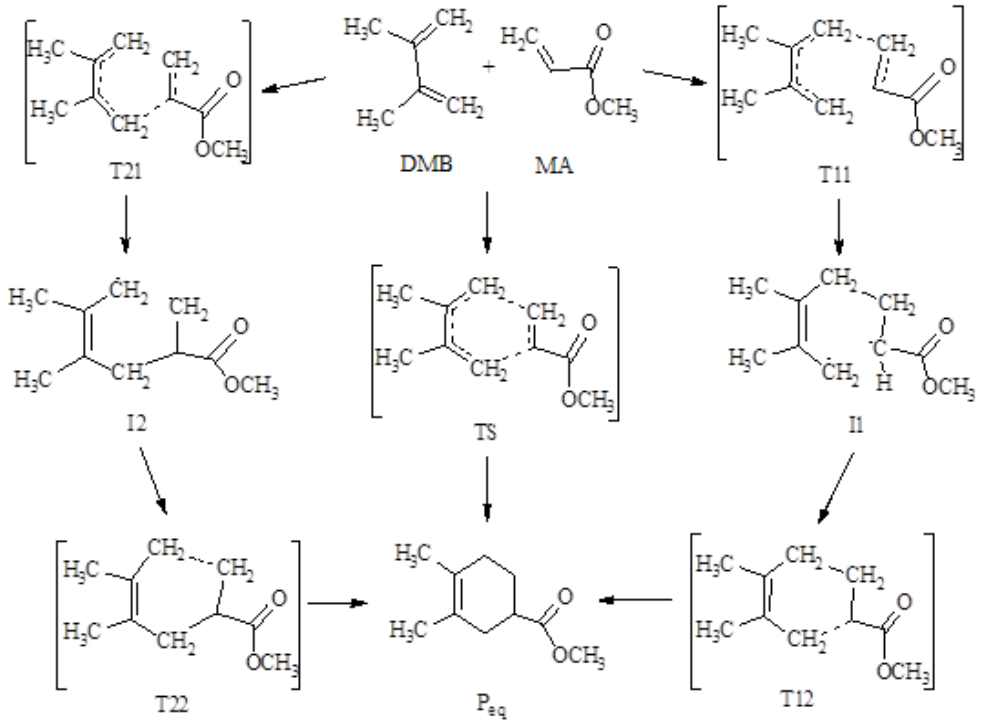
The quantum-chemical modeling of the reaction mechanism of 2,3-dimethylbuta-1,3-diene (DMB) and methyl acrylate (MA) [4+2]-cycloaddition was conducted by MOPAC2009 and semiempirical method RM1 [1]. It belongs to the electrocyclic reactions and can proceeds according to the concerted mechanism [2] in a one-step or two-step interaction [3].



The calculation results of the activation parameters and analysis the obtained potential energy surfaces using unrestricted and restricted Hartree-Fock indicate the passage of the process according to the concerted two-stage mechanism (UHF), rather than one-stage concerted mechanism with (RHF). With the passage of the two-stage process according to the concerted mechanism to overcome the energy barrier of the reaction requires less energy compared with one-stage interaction.

Literature:

1. Stewart, J.J.P. *Program Package MOPAC2009* (http://www.openmopac.net)

2. Jensen, F. Introduction to Computational Chemistry / F.Jensen // Wiley.- 2006.- p.620.

3. Brückner R. Hardcover Organic Mechanisms - Reactions, Stereochemistry and Synthesis / R. Brückner // First Edition. – 2010. - p. 856.