

# Epoxidation of 1-Substituted 3-Cyclohexenes. Theoretical and Experimental Investigation

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**Abstract**—Epoxidation of 1-substituted 3-cyclohexenes was investigated. The stereoisomeric composition of the forming epoxides mixture was established by means of GLC and  $^1\text{H}$  NMR spectroscopy. The spectral parameters of the epoxides are considered. The thermodynamical stability of *cis*- and *trans*-epoxides was evaluated by molecular mechanics method. For the epoxidation of 1-substituted 3-cyclohexenes with peracetic acid a quantum-chemical calculation of the potential energy surface by PM3 method was carried out.