A QUANTUM CHEMICAL STUDY OF 1,2,4-TRIAZINE REACTIVITY IN REACTIONS WITH ELECTROPHILIC AND NUCLEOPHILIC REAGENTS

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B3LYP/6-311+G(*d*,*p*) and MP2/6-31G(*d*,*p*) methods are used to study the electronic structure of a 1,2,4-triazine molecule. Quantitative characteristics of the reactivity are obtained in the form of atomic charges and Fukui coefficients. Thermodynamic characteristics are determined for the protonation reaction and addition of the hydride anion to a 1,2,4-triazine molecule.

Keywords: 1,2,4-triazine, density functional theory, electronic structure, Fukui coefficients, thermodynamic parameters.