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Quantum chemical interpretation of dipeptides and aminoacids reactivity in processes of acids amides and sulfamides formation

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Abstract

Quantum chemical simulation of aminoacids and dipeptides anions, as well as chloroanhydrides of benzoic, sulfobenzoic, 3-nitro-, 4-methylsulfobenzoic acids and nitro substituted phenyl esters of benzoic acids is carried out by ab initio methods. It is established that values of nitrogen atoms charges can be used as reactivity indexes of nucleophiles in *N*-acylation; acylation agents reactivity is connected with LUMO energies of their molecules. PES of glycine reaction with 4-methylbenzene sulfonyl chloride in gaseous phase is calculated, it is shown that the reaction occurs by S_N2 mechanism.