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Reactivity of α-alanine in arensulfonylation in aqueous-organic media: kinetic experiment and reaction root simulation

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Abstract

On a basis of experimental investigation of kinetics of *D,L-α-alanine* reaction with 3-nitrobenzenesulfonyl chloride in systems water–2-propanol and water–1,4-dioxane of a variable composition in polytermal conditions activation parameters of the process are determined and conclusions are made about influence of the solvent composition on its rate. Quantum chemical simulation of the reaction root in conditions of formation of alanine mono-, di- and trihydrates is carried out. It is shown that specific alanine solvation by water molecules influences significantly on the reaction energy profile.