

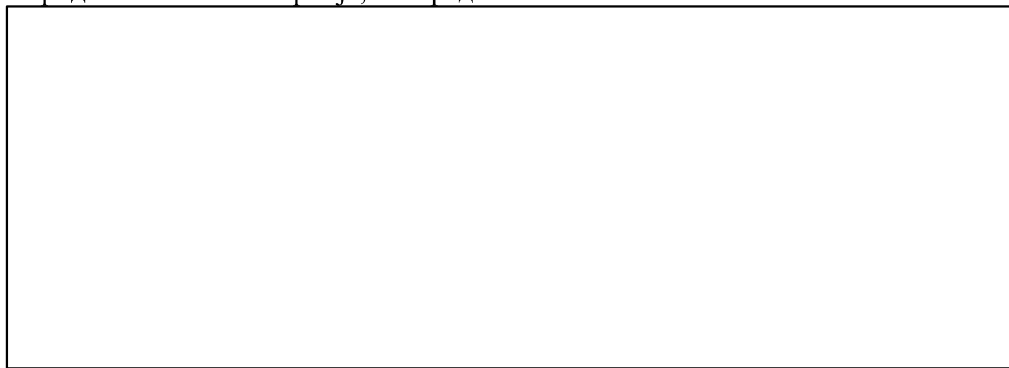
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Book of Abstracts

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The influence of solvent polarity on the kinetic and thermodynamic parameters of the reaction of substitution of methyl chloride with *p*-hydroxybenzoate anion

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This study investigates the influence of solvent polarity on the thermodynamic and kinetic parameters of the nucleophilic substitution reaction of methyl chloride with the *p*-hydroxybenzoate anion, which proceeds via the S_N2 mechanism [1]. The research aims to elucidate how various polar aprotic solvents, characterized by distinct dielectric constants, affect both the kinetics and thermodynamics of the reaction. The reaction was analyzed under vacuum conditions as well as in the presence of dimethyl sulfoxide ($\epsilon = 46.826$), dimethylformamide ($\epsilon = 37.219$), acetone ($\epsilon = 20.493$), and tetrahydrofuran ($\epsilon = 7.426$). Geometry optimization was done by using the M06-2X/6-311++G(d,p) theoretical model implemented in the Gaussian 09 software package, while the CPCM solvation model was applied to simulate the impact of the solvents [2]. By analyzing the reaction enthalpy (Δ_rH) and Gibbs free energy (Δ_rG), and calculating the reaction rate constant using Transition State Theory (TST) and Eyring's equation, it was determined that the substitution reaction became increasingly favorable, both kinetically and thermodynamically, with increasing solvent polarity. It is a consequence of the fact that polar aprotic solvents enhance the stabilization of both the transition state and the product complex. Symmetric polar aprotic solvents are highlighted as more suitable because their stabilization effect toward the product complex is higher. It is of significant importance when the leaving group is a small-volume anion, and then the stabilization of the product complex is enabled with the greater surface of the solvent's molecule positive charge.

References

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2. M. J. Frisch, G. W. Trucks, H. B. Schlegel, et. al, *Gaussian 09. Revision C.01*, **2010**, Gaussian Inc, Wallingford.

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