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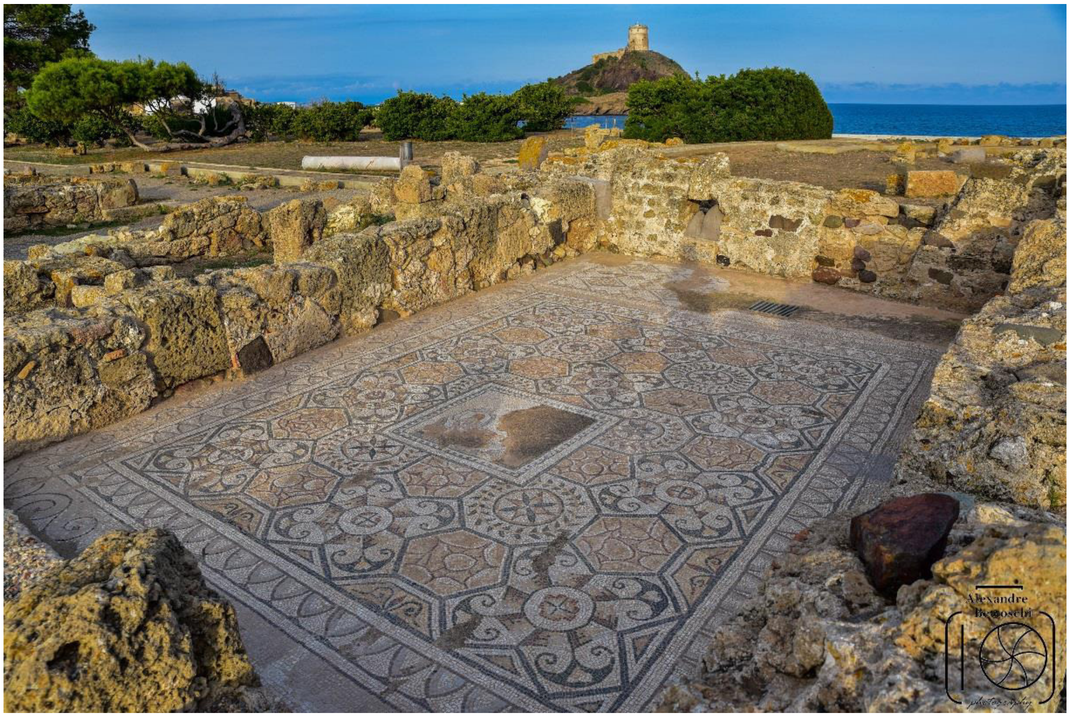

Book of Abstracts

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Solvent Effects on the Kinetics and Mechanism of Phenylselenoetherification of Some Δ^4 - Alkenols

Vera M. Divac, Marina D. Kostić, Kristina Z. Mihajlović, Zorica M. Bugarčić
Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia
veradivac@kg.ac.rs

Solvent-solute interactions can play a key role in organic synthesis. These interactions are commonly described as non-specific (van der Waals, dipole-dipole, etc.) and specific (hydrogen bonding). Through the solvation, reactants, reaction products or intermediates can be stabilized, but also these interactions can modify energy barriers thereby altering transition states and possible reaction pathways. Depending on the solvent, reaction rates can vary by orders of magnitude and as well as product distribution. Better understanding of solvent effects on the kinetics and mechanism of a reaction of interest can help to promote a desired reaction pathway or product by strategically choosing the appropriate solvent.

The aim of this work was to investigate the influence of solvent effects on the kinetics and mechanism of phenylselenoetherification of two isomeric (Z)- and (E)-hex-4-en-1-ols through the synthetic and kinetic study under pseudo-first order conditions by UV–Vis spectrophotometry. These two alkenols are chosen by their fascinating spectrum of possible products which differ by the used contra ion of reagent (Cl or Br) and the presence of base additive.[1, 2] The reactions were followed by varying reagents (PhSeCl or PhSeBr), presence of additive (in the presence or absence of pyridine) and in three different solvents (CCl4, THF and acetonitrile). The selected reaction media have diverse properties in terms of polarity and hydrogen bond capability which can be defined by the value of Gutmann's donor number (DN). By performing the reactions in these solvents and comparing the obtained results is allowing us to potentially isolate solvent effects which are beneficial for the cyclization reaction in terms of the kinetics and selectivity. The study have shown that rate constants are influenced both by the specific and non-specific interactions. While the increase of donor number of used solvent is favorable for the rate constant, the increase of solvent polarity is decreasing the reaction rate of cyclization.

References

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2. V.M. Divac, R. Puchta, Z.M. Bugarčić, *J. Phys. Chem. A,* 116, 7783-7790 (**2012**).