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NMR and UV-Vis Kinetic Study of the CoCl_2 -Catalyzed Phenylselenoetherification of Nerolidol

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Nerolidol represents acyclic sesquiterpene alkenol with rich medical potential, as well as with potential to serve as fragrant and flavor constituent in food.¹ Numerous biological activities have been expressed by the nerolidol, such as antimalarian, antiulcer and antiparasitic.² The phenylselenyl halide-induced oxyselenocyclization of the nerolidol present an important pathway for the synthesis of the substituted oxygen heterocycles (five- or six-membered cyclic ethers) which are structural subunits in many naturally occurring molecules.³ By the proper selection of the phenylselenyl halide reagent (PhSeCl or PhSeBr) and used catalyst (mild Lewis acids or Lewis bases), a satisfied results in terms of reaction yields and ratio of obtained cyclic ether products can be established. Although the oxyselenocyclization represent routinely used synthetic method, its kinetics and mechanism have not been sufficiently tested.

Therefore, herein we are presenting results of the NMR and UV-Vis kinetic studies on the CoCl_2 -mediated oxyselenocyclization of the nerolidol, by the use of PhSeBr as cyclization reagent. The reaction between nerolidol and PhSeBr , in the presence of equimolar amount of CoCl_2 affords exclusively organoselenium-functionalized five-membered cyclic ether in quantitative yield (100%). PhSeBr is better choice than PhSeCl for the NMR-kinetic part of the investigation, due to slower reaction rate which allowed us to easily monitor the process and acquire spectra at controlled time intervals. Another advantage of the NMR spectroscopy for the kinetic investigations is possibility to elucidate the structural changes during reaction. NMR kinetics was performed in CDCl_3 as a solvent and using equimolar amounts of the reactants (nerolidol, PhSeBr and CoCl_2 , 1:1:1), while UV-Vis kinetic part of the experiment was accomplished in THF, under *pseudo*-first order reaction conditions, where concentration of nerolidol was always in excess. The calculated values of the rate constants for the NMR and UV-Vis methods are showing good agreement and consistency between two applied methods. This is another proof of the NMR validity for the determination of the kinetic parameters and investigations of the reaction pathways.

References

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