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Kinetic and Mehanistic Studies of Pyridine-Catalyzed Selenolaktonization of 2-Cyclopentene-1-Acetic acid

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Abstract

Purpose

In addition to the wide range of reagents that can be used in intermolecular cyclization reactions of unsaturated substrates like alcohols, acids and amines, phenylselenyl halides represent very useful reagents due to the high stereoselectivity of these reactions as well as mild reaction conditions. (Denmark, 2006:71). The purpose of this research was to obtain synthetically very useful bicyclic lactone by intramolecular cyclization of 2-cyclopentene-1-acetic acetic acid by PhSeCl or PhSeBr as a reagent. Also the aim of this study was to improve the reaction yields and selectivity through optimization of reaction conditions and investigation of kinetic and mechanism of these reactions.

Design / Methodology / Approach

The intramolecular cyclization of 2-cyclopentene-1-acetic acid by PhSeCl or PhSeBr was performed in variety of solvents, at room temperature and in the presence and absence of some Lewis bases as additives. When the reaction conditions were optimized, the kinetic investigation was performed, where all reactions were monitored as pseudo-first order reactions in THF as a solvent by UV-Vis spectrophotometry at 288K in the presence and absence of pyridine.

Findings

The study have shown that the best results in terms of yields and selectivity was with the use of PhSeCl as a reagent and pyridine as an additive. There is a wide range of suitable solvents that can be use in these reactions, among which are THF, chloroform, methylenchlorid, diethyl ether and acetonitrile. The use of pyridine as an additive, resulted in almost quantitative yields with pronounced selectivity. Namely, it is noticed that course of the reaction goes through the 5-exo-trig cyclization proces while the 6-endo-trig product doesn't occur. The obtained values for rate constants have shown that the reactions with PhSeCl are almost twice faster than corresponding reactions with PhSeBr as a reagent. Also, the use of pyridine as

an additive, significantly accelerates the reactions compared to the reactions performed without the presence of additives.

Originality / Value

This research have shown the simple and efficient method for preparing the bicyclic compound in high yields and with pronounced stereoselectivity. The main gain of this study is the highly modular nature of obtained product which can be easily transformed in a wide range of functionalities as the removal of organoselenium group is simple with the possibility of formation substitution or elimination product. (Tiecco, 2000:41) Likevise, this research have confirmed the general princip of our previous studies on unsaturated alkohols. (Divac, 2012:116)

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