

عنوان مقاله:

Effect of Solvents on Kinetics and Mechanistic Investigation of Highly Substituted Piperidines: Spectrometry Approaches

محل انتشار:

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خلاصه مقاله:

On the basis of reaction rates, chemical equilibrium positions, competitive reaction mechanisms, chemoselectivity, and stereoselectivity, various solvent effects can be categorized. Most organic reactions fall into one of several categories, including dipolar transition state, isopolar transition state, nonpolar transition state, and others, depending on how sensitive to solvents they are. In this instance, kinetic considerations were made for the formation of substituted piperidine **1** from the reaction between **1**-methylbenzaldehyde **1**, aniline **2**, and ethyl acetoacetate **3** in the presence of oxalic acid dihydrate at room temperature in both methanol and ethanol media. In addition to being an excellent catalyst, oxalic acid dihydrate is a substance that is kind to the environment. To investigate the kinetics and mechanism of the aforementioned reaction, UV-vis spectrophotometry was used. The data from the experiment indicate that there are two steps in the reaction overall. The reaction was carried out multiple times at various temperatures and the relationship between the overall rate constant, $\ln k_{\text{ove}}$, or $(\ln k_{\text{ove}}/T)$, and the reciprocal temperature was well supported by the Arrhenius and Eyring equations, respectively. This gave the necessary plots to calculate the reaction's parameters (E_a , ΔS^\ddagger , ΔH^\ddagger , and ΔG^\ddagger). Methanol was previously recognized as a desirable solvent in the synthesis of piperidine. However, in a kinetic investigation, ethanol had good effects on accelerating the reaction rate compared with methanol. Ethanol is classified as an environmentally preferable green solvent because it is available by fermenting renewable sources, including sugars, starches, and lingo cellulose, while, methanol is a toxic alcohol. Herein, we have shown ability of ethanol as a solvent to synthesis of substituted piperidines. The outcomes demonstrated that step k_1 is a rate-determining step (RDS) in the reaction mechanism. The obtained results and the steady state approximation supported the proposed mechanism.

کلمات کلیدی:

Kinetic and Mechanistic Investigation Catalyst Oxalic acid dihydrate Multicomponent Reaction UV, vis spectrophotometry Piperidine

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