Organic Chemistry: An Indian Journal

Organic Chemistry
ISSN: 0974-7516

Short Commentary | Vol 15 Iss 1

Influence of Acoustic Vibrations on the Kinetics and Mechanism of First-Order Chemical Reactions in Nano-structured Liquid Phase

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Received: November 08, 2018; **Accepted:** November 22, 2018; **Published:** December 02, 2018

Introduction

As is known [1-3], acoustic vibrations (10-100 Hz) may affect the kinetics of chemical reactions in some specific conditions [1,3]. In this work, we modeled the impact of acoustic vibrations on the rate of first or second-order liquid-phase reactions with due regard for the formation of associates.

The scheme of the first-order reaction yielding product B from monomers A_1 and dimers A_2 can be written [1,4] as:

Mathematical Model

$$A_1 \rightarrow B, \qquad k_1 \qquad (1)$$

$$A_2 \rightarrow B + A_1, \qquad k_2 \qquad (2)$$

$$2A_1 \leftrightarrow A_2, \qquad K \qquad (3)$$

Where K is the equilibrium constant.

Accordingly, the expression for reaction rate w acquires the form [1]:

$$W=k_{ef}[A]=K^{-1}k_1[(0.0625+0.5K[A])^{0.5}-0.25]+K^{-1}k_2[(0.0625+0.5K[A])^{0.5}-0.25]^2 \quad (4)$$

Citation: Kulagina TP, Smirnov LP, Chegodaev NA. Influence of Acoustic Vibrations on the Kinetics and Mechanism of First-Order Chemical Reactions in Nano-structured Liquid Phase. Org Chem Ind J. 2018;15(1):132

The strain/compression waves induced in the solution by acoustic waves of frequency ν affect the equilibrium constant $K_\nu(t)$ for dissociation of the associates. According to Chegodaev NA et al., and Kulagina TP et al. [4,5], the latter can be written in the form:

$$K_\nu(t)=K_0 \exp[-P_0 \sin(2\pi\nu t)], \quad (5)$$

Where K_0 is the equilibrium constant without the external action, P_0 is the amplitude of applied field.

Rate constant w was found to depend on k_1, k_2, and monomer/dimer ratio (**FIG. 1**). The influence of acoustic wave with angular frequency $\omega=2\pi\nu$ was calculated from formula (5) under the assumption that equilibrium constant $K_\nu(t)$ can be used as averaged value K_{av}:

$$K_{av} = \int_0^{t_c} K_\nu(t)dt/t_c, \quad (6)$$

Where $tc=(2\pi\nu)^{-1}$ is the period of action. The dependence of relative reaction rate Δw on [A] is exemplified in **FIG. 1**. Here $\Delta w=(w-w_\nu)/w$, where w_ν is reaction rate (4) at $K_0=0.2$, $K=K_{av}$ (6), $\omega=18.84\ s^{-1}$, and $P_0=15$.

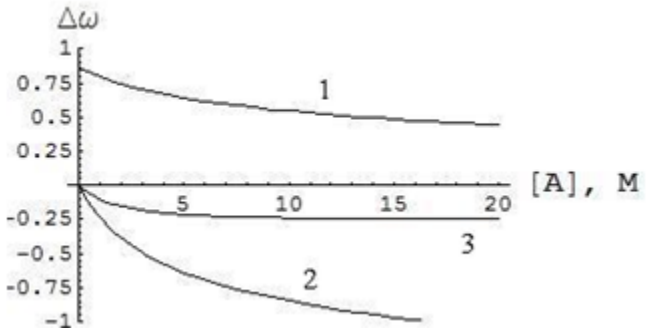

FIG. 1. **Relative reaction rate Δw as a function of [A] for: $k_1=0$, $k_2=5$ (1); $k_1=5$, $k_2=0$ (2), and $k_1=5$, $k_2=5$ (3).**

As follows from **FIG. 1**, the reaction kinetics is defined by the reactivity of monomers and dimers. The reaction rate increases when the reactivity of dimers is higher than that of monomers, and vice versa. From **FIG. 1** it is visible that the reaction does not depend on a ratio of rate constants k_1 and k_2 and also reaches an extreme value at high concentrations. The influence of mechanical action depends on its amplitude and is independent of its frequency. The connection of chemical reaction rate and concentration of reagents with parameters of wave mechanical influence (amplitude, oscillation frequency) also depends on the kinetic scheme of reaction and supra-molecular structure of reagents (quantity and type of associates).

This work was financially supported by FASO (grant 0089-2014-0021).

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