

Abstract

The kinetics of epoxidation of 4-fluorochalcone, 4-nitrochalcone, and 4-chlorochalcone in a single-phase system consists of water/acetonitrile/ethyl methyl imidazolium bromide was explored. The system had the following reactants: a substituted chalcone, an oxidant (hydrogen peroxide), and a base (sodium hydroxide). The overall rate laws for each of the substituted chalcones (4-fluorochalcone, 4-nitrochalcone, and 4-chlorochalcone) are the following:

$$\text{rate (M/sec)} = 0.00185[4 - \text{Fluorochalcone}]^{0.4716}[\text{NaOH}]^{1.1408}[\text{H}_2\text{O}_2]^{0.4095}$$

$$\text{rate (M/sec)} = 53.54[4 - \text{Nitrochalcone}]^{1.1408}[\text{NaOH}]^{0.8206}[\text{H}_2\text{O}_2]^{0.4466}$$

$$\text{rate (M/sec)} = 0.570[4 - \text{Chlorochalcone}]^{0.7392}[\text{NaOH}]^{1.5192}[\text{H}_2\text{O}_2]^{0.6153}$$

The rate constants were calculated to be $0.00185 \pm 0.00098 \text{ M}^{-1.0219}\text{sec}^{-1}$, $53.54 \pm 21.94 \text{ M}^{-1.7953}\text{sec}^{-1}$, and $0.570 \pm 0.318 \text{ M}^{-1.8737}\text{sec}^{-1}$ for 4-fluorochalcone, 4-nitrochalcone, 4-chlorochalcone, respectively. The activation energies were determined to be 74.74 kJ/mol, 64.81 kJ/mol, and 54.68 kJ/mol for 4-fluorochalcone, 4-nitrochalcone, and 4-chlorochalcone, respectively. The pre-exponential factors were determined to be $1.98 \times 10^{10} \text{ M}^{-1.0219}\text{sec}^{-1}$, $1.03 \times 10^{13} \text{ M}^{-1.7953}\text{sec}^{-1}$, and $1.77 \times 10^9 \text{ M}^{-1.8737}\text{sec}^{-1}$ for 4-fluorochalcone, 4-nitrochalcone, and 4-chlorochalcone, respectively. The rate constants for substituted chalcones were significantly higher than the rate constant calculated in a study with a biphasic system. However, the activation energy was determined to be higher when compared to the biphasic system. The reaction constant (ρ) for the epoxidation reaction was determined to be 5.8708, indicating that the reaction was aided by the presence of an electron withdrawing group.