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ORIGINAL ARTICLE

Hydrophobicity and kinetic inspection of hydroxide ion attack on some chromen-2-one laser dyes in binary aqueous–methanol and aqueous–acetone mixtures: Initial state-transition state analysis

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Abstract In the present study, reactivity base-catalyzed hydrolysis of 7-dimethylamino-4-methyl-2H-chromen-2-one (DMAC) and 7-diethylamino-4-methyl-2H-chromen-2-one (DEAC) in binary aqueous–methanol and aqueous–acetone mixtures was examined at 298 K. Kinetic results, rate laws and reaction mechanisms were established. Moreover, the change in the activation energy barrier of the investigated compounds from water to water–methanol and water–acetone mixtures was estimated from the kinetic data. Base-catalyzed hydrolysis of (DMAC) and (DEAC) in aqueous–methanol and aqueous–acetone mixtures follows a rate law with $k_{obs} = k_2[OH]$. The decrease in the rate constants of (DMAC) and (DEAC) as the proportion of methanol and acetone is due to the destabilization of OH^- ion. The solubilities of the studied compounds, DMAC and DEAC in water–methanol and water–acetone mixtures were established and their transfer chemical potentials were calculated. Solvent effect on reactivity trends of the investigated compounds has been analyzed into initial and transition state components by using the transfer chemical potentials of the reactants and the kinetic data of the studied compounds. The decrease in the observed rate constant values (k_{obs}) of the base hydrolysis of DMAC and DEAC with increasing of methanol% or acetone% is dominated by the initial state (IS).

1. Introduction

Coumarins belong to a group of compounds known as the benzopyrones, all of which consist of a benzene ring joined to a pyrone. Coumarin and the other members of the coumarin family are benzo-α-pyrones, while the other main members of the benzopyrone group, the flavonoids contain the γ-pyrone group (Ramazani et al., 2008; Khoobi et al., 2012; Zareai et al., 2012).

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