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Evaluation of the interaction between molecules during betaine monohydrate-organic acid deep eutectic mixture formation

Ida Zahrina^{1,2}, Mohammad Nasikin, Kamarza Mulia^{1*}

Abstract

Deep eutectic solvents (DES) are attractive as green media because DES are non-toxic and biodegradable. DES are obtained by mixing a quaternary ammonium salt with a hydrogen bond donor (HBD) until they form a eutectic mixture. Recently, DES have been widely applied as solvents for extraction processes. Because the solutes and HBD competitively interact with salt during the extraction process, the stability and strength of the interaction between salt and HBD molecules on DES formation should be evaluated. In this study, the interactions between molecules of the betaine monohydrate salt and different HBDs consisting of liquid organic acids (*i.e.*, propionic and acetic acid) in eutectic mixture formation were investigated by thermodynamic and spectroscopic analyses. On the basis of thermodynamic analysis, the stability and strength of the molecular interaction between betaine monohydrate and propionic acid was greater than the stability and strength of the molecular interaction between betaine monohydrate and propionic acid molecules was - 15.7 kJ.mol $^{-1}$, with an excess Gibbs free energy (G^E) of 0.81 kJ.mol $^{-1}$ at the eutectic composition. The spectroscopic analysis indicates the presence of a weak interaction between the betaine monohydrate and acid molecules.

Keywords: betain monohydrate, DES, molecular interaction, organic acid, stability and strength

1. Introduction

Deep eutectic solvents (DES) have attractive physicochemical properties such as a lack of volatility, thermal stability, non-flammability, high conductivity, and good solubilizing capacity for organic or inorganic compounds [1], and are thus suitable for use as green media. Likewise, DES have been applied in many applications, such as a catalyst for media reactions [2–5] and

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