Experimental and Quantum Chemical Calculation for the Production of High Purity of Ethyl Acetate

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Abstract

Densities of pure ethanol, acetic acid, ethyl acetate, water, 1-ethyl-3-methylimidazolium hydrogen sulphate {[EMIM][HSO4]},1-ethyl-3-methylimidazolium ethylsulphate {[EMIM][EtSO4]}, choline chloride glycerol {[ChCl][Gly] and choline chloride acetic acid {[ChCl][AA]} and their binary mixtures were measured over the entire composition range at different temperatures from 293.15 K to 343.15 K. Volumetric properties including molar volume, excess molar volume, partial molar volume, excess partial molar volume, apparent molar volume, isobaric expansivity and excess isobaric expansivity were calculated from this measured density data. Further, the sigma profile and sigma potential of all the studied components were generated using COSMO-RS Model. Finally, the green esterification of ethanol with acetic acid in the presence of 1-ethyl-3-methylimidazolium hydrogen sulphate [EMIM][HSO4] as potential catalyst media were conducted at 298.15 K. The reactant and catalyst ratio were chosen and taken as 7:4 and thereby achieved 80.96% yield.

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