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Kinetic and thermodynamic studies on one-step synthesis of methyl acrylate promoted by generated ionic liquid at mild temperature

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Abstract: One-step aldol condensation of methyl acetate with formaldehyde (or trioxane) for preparing methyl acrylate at 623 K-653 K has stimulated researchers' attention in recent years. Herein, a new methodology for one-step synthesis of methyl acrylate from methyl acetate and trioxane promoted by generated trifluoromethanesulfonate ionic liquid, *via* aldol condensation, at mild temperature was developed. The kinetic and thermodynamic studies on this new process were also firstly investigated systematically. Experiments were conducted in a batch reactor under the temperatures of 283 K-298 K and reaction times of 10 min-100 min, wherein the side reactions could be ignored. The proposed mechanism-based kinetic model was established and simulated with experimental data. The model showed good agreement with experimental results within the range of acceptable deviation, thereby the pre-exponential factor and activation energy of each reaction step were obtained. Moreover, the equilibrium constant and enthalpy change of each reversible reaction were also calculated through Van't Hoff formula.

Keywords: Aldol condensation; Methyl acrylate; Ionic liquid; Kinetic; Thermodynamic

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