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Integrated Two Stage Processing of Biomass Conversion to Hydroxymethylfurfural Esters Using Ionic Liquid as Green Solvent and Catalyst: Synthesis of Mono Esters

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Abstract: In this study, a two-stage process was established for the synthesis of HMF esters using ionic liquid acid catalyst. Ionic liquid catalyst with different strength of the Bronsted acidity was prepared in the laboratory and characterized using 1H NMR, FT-IR, and 13C NMR spectroscopy. Solid acid catalyst from the ionic liquid catalyst was prepared using the immobilization method. The acidity of the synthesized acid catalyst was measured using Hammett function and titration method. Catalytic performance was evaluated for the biomass conversion to 5-hydroxymethylfurfural (5-HMF) and levulinic acid (LA) in methyl isobutyl ketone (MIBK)-water biphasic system. A good yield of 5-HMF and LA was found at the different composition of MIBK: Water. In the case of MIBK: Water ratio 10:1, good yield of 5-HMF was observed at ambient temperature 150°C. Upgrading of 5-HMF into monoesters from the reaction of 5-HMF and reactants using biomass-derived monoacid were performed. Ionic liquid catalyst with -SO₃H functional group was found to be best efficient in comparative of a solid acid catalyst for the esterification reaction and biomass conversion. A good yield of 5-HMF esters with high 5-HMF conversion was found to be at 105°C using the best active catalyst. In this process, process A was the hydrothermal conversion of cellulose and monomer into 5-HMF and LA using acid catalyst. And the process B was the esterification followed by using similar acid catalyst. All monoesters of 5-HMF synthesized here can be used in chemical, cross linker for adhesive or coatings and pharmaceutical industry. A theoretical density functional theory (DFT) study for the optimization of the ionic liquid structure was performed using the Gaussian 09 program to find out the minimum energy configuration of ionic liquid catalyst.

Keywords: biomass conversion, 5-HMF, Ionic liquid, HMF ester

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