



Energy Transition
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ETRI 2023

BOOK OF ABSTRACTS



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molecules using supercritical CO₂ and palladium-rhenium as a catalyst. The use of CO₂-SC as a reaction medium facilitated the selective production of economically important products for the chemical industry from the catalytic hydrogenation of fumaric acid (Ac.FUM), acting as a modulator of catalytic properties, similar to the use of the solvent MeOH. Its use promoted the formation of THF as a product.

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Abstract Title: Synthesis of New Polyurethanes from Biomass-derived Monomers

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Abstract: Polyurethanes (PU) are an interesting class of polymeric materials extensively employed in a variety of industries. Conventionally, they are synthesized by the polyaddition reaction between polyols and diisocyanates, typically from petroleum-derived sources. The work presented herein showcases the synthesis of new PU using biomass-derived monomers. Four new diols were obtained in good yields from 5-(chloromethyl)furfural or CMF (an interesting carbohydrate-derived platform molecule) and dithiols. Subsequently, the polyaddition reaction between these new diols and different diisocyanates was carried out employing organocatalysis as an alternative to the conventional tin-based catalysts.

Keywords: Biomass, Polyurethanes, 5-(chloromethyl)furfural.

Introduction and Objectives: Polyurethanes (PU) are an important class of polymeric materials used in several industries as foams, coatings, elastomers, and more. Their synthesis is conventionally performed by the polyaddition reaction between diols and bis-isocyanates monomers in the presence of some catalyst. However, these raw materials are predominantly derived from petroleum-based sources. An alternative approach to prepare these monomers is the use of biomass-derived platforms. For example, 5-(chloromethyl)furfural (CMF), which is easily prepared from fructose, has become an interesting substrate for the synthesis of monomers, fuels, and sustainable chemicals. In this work, CMF was employed as the starting material for the synthesis of new polyurethanes containing sulfur in their structure. Additionally, the polyaddition reaction was studied by employing organocatalysis (for example, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)) as an interesting alternative to the use of tin-based catalysts, which are difficult to remove from the PU and has high costs.

Methodology: Synthesis of PU from biomass-derived monomers Initially, the nucleophilic substitution reaction between CMF and dithiols was carried out in the presence of triethylamine

and tetrabutylammonium iodide giving the corresponding dialdehydes as the key intermediates. Then, these intermediates reacted with sodium borohydride, providing the desired diols. Four new compounds were obtained using this protocol. Subsequently, the polyaddition reaction between these diols was studied using different diisocyanates and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) as the catalyst.

Preliminary results: A new method to synthesize diol monomers, containing sulfur atoms, was developed from fructose. Twelve new polyurethanes were synthesized by the polymerization reaction between these diols and commercially available diisocyanates. All the polymers were well characterized using nuclear magnetic resonance (RMN), infrared spectroscopy (IR), and thermal gravimetric analysis (TGA).

Preliminary conclusions: New protocol for the synthesis of different diol monomers, containing sulfur atoms, was developed under mild reaction conditions from fructose. These diols were also employed for the synthesis of new biobased polyurethanes by the polyaddition reaction with commercially available diisocyanates.

Giovanni Rodrigues Morselli

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Abstract Title: Interactions between CO₂ and superbase in ionic liquids probed by vibrational spectroscopy

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Abstract: Alternative solvents are currently being investigated as media to capture and convert carbon dioxide (CO₂), given the corrosive, toxic and volatile properties of traditional amine aqueous solutions used in the CO₂ scrubbing process. Ionic Liquids (ILs) are a highlighted class of solvents exhibiting properties as non-volatility, non-flammability and a wide solvent capacity. To enhance CO₂ capture efficiency, ILs can be functionalized by incorporating task-specific moieties into their molecular structure or by mixing them with a task-specific compound, such as a superbase - a class of reactive nitrogen bases which are unstable in its pure form or in aqueous solutions. Therefore, the main objectives of this work are: to efficiently capture CO₂ by functionalizing ILs through the mixture with the superbase DBU (1,8