



## 7<sup>TH</sup> PORTUGUESE YOUNG CHEMISTS MEETING

# BOOK OF ABSTRACTS

**19<sup>th</sup> - 21<sup>st</sup> May 2021**

**Bragança - Portugal**

### Physical chemistry

- PC136** | Partitioning and solubility of phenolic compounds using the abraham solvation model  
*Isabella W. Cordova*
- PC137** | A supramolecular multiresponsive ternary complex  
*André Seco*
- PC138** | Modulation of the photochemical reactivity of a bischalcone upon complexation with cucurbit[7]uril  
*Rita Anastácio*
- PC139** | Fluorescent sensing of guanosines in water: a combination of complementary hydrogen bonds and electrostatic interactions  
*Artur J. Moro*
- PC140** | Polymorphism of 1-methylhydantoin investigation by periodic DFT calculations and characterization of the third polymorph  
*Bernardo A. Nogueira*
- PC141** | Supramolecular light-controlled counterion activator for the transport of cationic peptides  
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### Surface chemistry and interfaces

- PC142** | *Agapanthus africanus*: a source of inspiration for the preparation of superhydrophobic hybrid films  
*P. Nunes*

### Other research areas

- PC143** | Kinetic study of biodiesel production using choline hydroxide as catalyst  
*Khadidja Hachemane*
- PC144** | The risk of emerging mycotoxins in the maize food chain  
*Marta Leite*
- PC145** | Exploring tazobactam for the development of antibiotic coordination frameworks by mechanochemistry  
*Daniela R. Ferreira*

## KINETIC STUDY OF BIODIESEL PRODUCTION USING CHOLINE HYDROXIDE AS CATALYST

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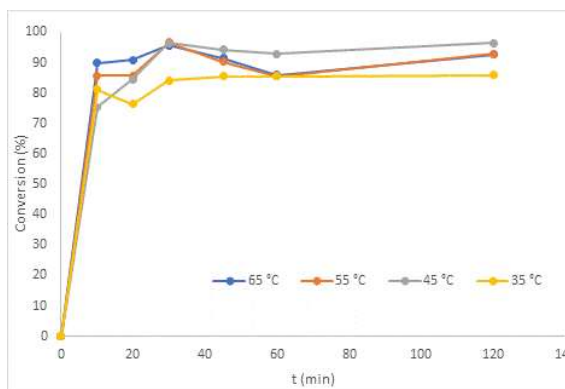
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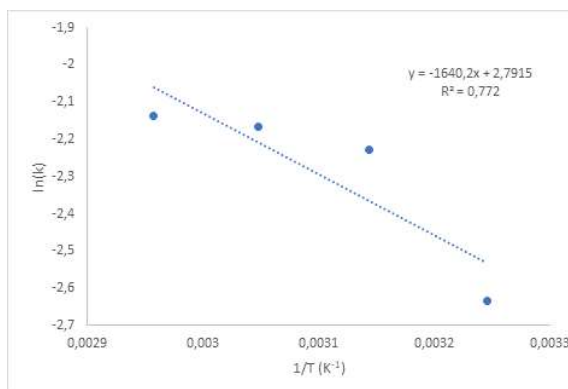
Due to the finite stock of fossil fuels and its negative impact on the environment, many countries across the world are now leaning toward renewable sources energies like solar energy, wind energy, biofuel, hydropower, geothermal and ocean energy to ensure energy for the society development security. Biodiesel is one type of biofuel that is renewable, biodegradable and has similar properties of fossil diesel fuels [1].

Biodiesel is a mixture of fatty acids methyl esters (FAMES) and can be produced through esterification of fatty acid mixtures or transesterification of vegetable oils and animal fats, using homogeneous and heterogeneous catalysts. Ionic liquid (IL) based catalysts are more and more used since they can be recovered and reused and can have the ability to catalyze both esterification and transesterification reactions. Thus, these types of catalysts, represent clear environmental and safety advantages in relation to classical catalysts.

The present work aims to study the use of choline hydroxide IL (ChOH) as a potentially reusable catalyst for the production of biodiesel. A kinetic study was carried out for the transesterification of a previously characterized vegetable oil sample [2], with methanol, under the specific conditions: 2 wt.% catalyst dosage, 1:10 oil/methanol molar ratio, for the reaction times of 10, 20, 30, 45, 60 and 120 minutes at 65, 55, 45, and 35 °C (*vd.* Fig.1). Transesterification with ChOH provided a 95.7% conversion in FAME content for 30 min of reaction at 65 °C. The results of the kinetic study demonstrated that the first-order model was generally the best fit for the reaction kinetics considering all the temperatures, with a rate constant (*k*) estimated as 0.1182 min<sup>-1</sup> for 65 °C, and an estimated activation energy of 13.64 kJ/mol (*vd.* Fig.2).



**Figure 1:** Conversion time evolution curves for oil:alcohol molar ratio = 1:10, % catalyst = 2 (wt/wt).



**Figure 2:** Estimation of the activation energy through the Arrhenius equation.

### References

- [1] H.M. Mahmudul, F.Y. Hagos, R. Mamat, A. Abdul Adam, W.F.W. Ishak, R. Alenezi, Renewable and Sustainable Energy Reviews 72 (2017) 497–509.
- [2] R. Lima, A.K.C.L. Lobato, A. Queiroz, A. E. Ribeiro, P. Brito, XXV Encontro Galego-Português de Química, Santiago de Compostela, Espanha, 2019.