GLOBAL E-CONFERECE ON
CHEMISTRY AND CHEMICAL ENGINEERING
APRIL 05-06, 2023 | WEBINAR

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Computational Studies of Biomass Residues Purification: Elimination of Oxygen from Oxolane and its Monomethylated Derivatives through Hydrodesoxygenation Process

The continuing demand of fossil fuels has focused considerable attention on the development of new fuel sources to replace non-renewable fossil fuels. One of such green fuel sources is biomass, which is appropriate to produce clean alternative fuel instead of non-renewable ones. However, the high oxygen content of organic compounds in biomass creates several undesirable properties in biofuels, such as low energy density, instability, high viscosity and corrosion on contact surfaces. Therefore, various upgrading techniques have been developed for the valorisation of biofuels with emphasis on the hydrodeoxygenation (HDO) process. In this report, the organic residues Oxolane and its Monomethylated Derivatives (2-Methyloxolane and 3-Methyloxolane) are treated by adsorption and catalytic hydrogenolysis (HDL) for removal of the oxygen heteroatom to get an expected purity of these compounds. The mechanisms are explained via DFT calculations at B3LYP/6-31G(d) method for the reactions without catalysts and LanL2DZ/6-31G(d) with catalyst. Each molecule was subjected to both successive hydrogenolysis, in presence and absence of catalyst at a temperature of 523 K and pressure of 40 bars. Variations in the geometric, thermodynamic and kinetic parameters are calculated to examine the whole processes. Each of these molecules underwent ring opening by heterolytic disruption of one of the C-O bonds in the first and second hydrogenolysis followed by removal of a water molecule by disruption of the second C-O bond. The first hydrogenolysis produced an alcohol (Butan-1-ol, Pentan-1-ol, 3-Methylbutan-1-ol) reaction intermediate and the second hydrogenolysis resulted in the formation of an alkane (Butane, Pentane, 3-Methylbutane) at each step during reaction.

Keywords: Oxolane Derivatives; Activation energy (Ea); Hydrodeoxygenation; DFT; Biomass.

Biography:

Dr. Simplice Koudjina, has been working as an Assistant Professor in Computational Theoretical Chemistry and Molecular Surface Modeling for Nanotechnology Applications at the National University of Sciences, Technology, Engineering and Mathematics (UNSTIM) in Benin, where he works since 2018. He holds a Ph.D. degree in Theoretical Chemistry and Molecular Surface Modeling at the University of Abomey-Calavi since 2016. He obtained M.Sc. in Nanotechnology at the University of Namur in Belgium. He then joined the research group of Professor. Guy Sylvain Y. Atohoun in the Unit Theoretical Chemistry and Molecular Modeling (UCT2M) at University of Abomey-Calavi (UAC) in BENIN. At 2022, he has obtained a PostDoc research stay in the group of Professor. Prabhakar Chetti in Department of Chemistry at National Institute of Technology (NIT) Kurukshtra – INDIA. His field of expertise is computational Chemistry and Molecular Surface Modeling. He has published more than 25 research articles in impact factor journal.

doi.org/10.51219/URForum.2023.Simplice-KOUDJINA ISBN-978-1-7393132-7-2