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Entitled

CATALYZED SELECTIVE FORMATION OF BXT COMPOUNDS FROM CATALYTIC HYDRODEOXYGENATION OF DATE PITS: A COMBINED EXPERIMENTAL-THEORETICAL INVESTIGATION

By

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Abstract

Date palm (Phoenix dactylifera) pits constitute an important category of waste biomass in many parts of the world. The main aim of this thesis is the use of surface-assisted hydro-deoxygenation reactions via different catalysts, to convert typically oxygenated pyrolysates of biomass oil extracted from date pits into transportation fuels. The main pyrolysis experiment, in conjunction with the hydro-deoxygenation experiments, were performed using a pyrolysis reactor at the following ranges of temperatures: 100°C–200°C, 200°C–300°C, 300°C–400°C, and 400°C–500°C, and products were collected and analyzed using GC/MS and FTIR. The selected catalysts (Nickel-supported-Beta zeolite and Cobalt-supported with molybdenum disulfide) were both tested for the hydrodeoxygenation processes. It was found that the Nickel-supported zeolite catalyst exhibited a higher conversion and selectivity towards BTX (benzene, toluene, xylene) products, than the sulfided cobalt catalyst. In particular, the highest conversion towards the product Toluene using Ni/H-Beta was attained in the condensable range of products between 300 – 400 °C, at 63.87 %. Additionally, density functional theory calculations (DFT) were used to map out decomposition mechanisms of several model compounds found in the date pit, such as maltol, 2-morpholinecarboxamide and vanillin. Likewise, DFT calculations were used to develop a mechanism for the surface-assisted hydrogenation reactions. Outcomes from the thesis shall be useful in efforts that target conversion of waste biomass into fuel fractions in semi-arid regions where conventional types of biomass are rather scarce.

Keywords: Pyrolysis, date pits, pyrolytic products, hydrodeoxygenation reactions, GC/MS, selectivity, conversion, density functional theory calculations.