ISGC 2022

N°1513 / PC
TOPIC(s) : Biomass conversion / Polymers or composites

Theoretical study of furfural derivatives reactivity/selectivity with alkynes: towards a potent valorisation route

AUTHORS

Richail Dubien MOULANDOU-KOUMBA / UNIVERSITE DE POITIERS, 4 RUE MICHEL BRUNET, POITIERS
Frédéric GUENGAN / UNIVERSITE DE POITIERS, 4 RUE MICHEL BRUNET, POITIERS
Samuel N'SIKABAKA / UNIVERSITE MARIEN NGOUABI, AVENUE DES PREMIERS JEUX AFRICAINS, DIATA, BRAZZAVILLE
Gilles FRAPPER / UNIVERSITE DE POITIERS, 4 RUE MICHEL BRUNET, POITIERS

PURPOSE OF THE ABSTRACT

The development of new technologies allowing access to biosourced molecules of interest according to more atomic, water and energy efficient processes has become a major industrial, environmental and societal challenge. Furfural is one of the compounds produced on a large scale from lignocellulosic biomass waste, and at an attractive market price (1.5-2.5 ?/kg), making this molecule a strategic synthon for the manufacture of bio-based products. The synthesis of renewable aromatics (BTX) from bio-based furfural derivatives and cheap alkynes is achieved using a Diels-Alder/aromatisation sequence. Predicting the reactivity and controlling the ortho/meta selectivity in the Diels-Alder step is an important issue to pave the way for a wide range of renewable oxygenated aromatics, but it remains a challenging task. Theoretical studies reveal that, in general, the ortho and meta ring charge products are the kinetic and thermodynamic products, respectively. The nature of the substituents, both on dienes and dienophiles, has a significant impact on the feasibility of the reaction, through modulation on the nucleo and electrophilic character of the reactants, as well as on the ortho/meta ratio. We show that the ortho/meta selectivity at reaction equilibrium comes from two antagonistic factors, charge interactions, favouring ortho products, and steric interactions, favouring meta products. This work also shows a more optimised pathway than that of ethylenic derivatives.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

Biomass | aromatics | DFT | Furfural

BIBLIOGRAPHY

[1] Scodeller, I v,. De Oliveira Vigier, K,. Muller, E,. Ma, C,. Guégan, F,. Wischert, R,. and Jérôme, F,. ChemSusChem 2021, 14, 313 -323.

[2] Avérous, L., & Caillol, S. L'Actualité Chimique, Société chimique de France, 2021, .95-100. hal-03058563