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Poster abstract

WP n°: 3

Title: Selectivity prediction for the citronellal cyclization on various catalysts

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Summary (max 200 words)**:**

Recently, the spectrum of nanoporous materials such as zeolites and zeotype structures has been further expanded through the discovery of a new class of hybrid porous solids [1]. Those materials, nowadays also known as metal organic frameworks or MOFs, consist of both inorganic and organic moieties. Certain MOFs exhibit a very interesting adsorption and even catalytic behavior [2]. In this study, the citronellal cyclization is investigated on industrially relevant homogeneous catalysts, such as $ZnBr_2$ and ATPH, but also on heterogeneous MOF catalysts such as Cu_3BTC_2 and UiO-66. This Lewis catalyzed reaction leads to a product distribution of four isomers, with isopulegol as the most desired product as it can be hydrogenated to menthol. All possible reaction routes leading to the various isopulegol isomers are determined theoretically on extended cluster models constructed for each catalyst. In this way, theoretical selectivities are calculated and verified with experimental data.

[1] Ferey, G., Chemical Society Reviews 37 (2008) 191.
[2] Czaja, A. U., Trukhan, N. and Muller, U., Chem. Soc. Rev. 38 (2009) 1284.