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Poster abstract

WP n°: 3

Title: Modeling citronellal cyclization in Cu_3BTC_2 and UiO-66

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Summary (max 200 words)**:**

Recently, the spectrum of nanoporous materials like 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]. This study concerns the modeling of different Lewis acid catalyzed reactions in various MOFs: Cu connected with 1,3,5-benzenetricarboxylate linkers (Cu_3BTC_2) and an $Zr_6O_4(OH)_4$ octahedron connected with (amino-)terephtalate linkers (both UiO-66 and UiO-66(NH_2)). The cyclization of citronellal, already tested experimentally on Cu_3BTC_2, was taken as the first probe reaction [3]. The desired cyclization product is isopulegol, which can be hydrogenated to menthol. Possible reaction routes leading to the various isopulegol isomers are studied from theoretical viewpoint on Cu_3BTC_2 and UiO-66. The theoretically obtained selectivities on small MOF-clusters could already validate those promising experimental trends.

[1] Ferey, G., Chemical Society Reviews 37 (2008) 191.
[2] Czaja, A. U., Trukhan, N. and Muller, U., Chem. Soc. Rev. 38 (2009) 1284.
[3] Alaerts, L., Seguin, E., Poelman, H., Thibault-Starzyk, F., Jacobs, P. A. and De Vos, D. E. Chem.-Eur. J. 12 (2006) 7353.

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