

**WP n°: 3**

**Title:** Modeling citronellal cyclization in Cu<sub>3</sub>BTC<sub>2</sub> 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<sub>3</sub>BTC<sub>2</sub>) and an Zr<sub>6</sub>O<sub>4</sub>(OH)<sub>4</sub> octahedron connected with (amino-)terephthalate linkers (both UiO-66 and UiO-66(NH<sub>2</sub>)). The cyclization of citronellal, already tested experimentally on Cu<sub>3</sub>BTC<sub>2</sub>, 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<sub>3</sub>BTC<sub>2</sub> 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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