

Poster abstract

WP n°: 3

Title: Electronic effects of ligand substitution on Lewis acid catalysis with metal-organic frameworks

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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 towards isopulegol is investigated on the UiO-66, an $Zr_6O_4(OH)_4$ octahedron connected with terephthalate linkers. The experimental activity of this material for Lewis acid catalysis can be increased if nitro-terephthalate linkers are used during the synthesis. Extended cluster models are constructed and reaction possibilities are modeled on the UiO-66 and the UiO-66(NO₂) to verify this electronic modulation effect. As the experimental acceleration effect was reproduced theoretically, the ultimate clue was provided to unravel the nature of the active sites within those materials.

[1] Ferey, G., Chemical Society Reviews 37 (2008) 191.

[2] Czaja, A. U., Trukhan, N. and Muller, U., Chem. Soc. Rev. 38 (2009) 1284.