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Effect of linker substituents on the epoxidation performance of V-MIL-47

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Recently, the catalytic behavior of MOFs for various oxidation reactions has been investigated [1]. MOFs have the potential to eventually replace certain homogenous catalysts if they are tweaked in an intelligent way. In this contribution we will discuss the catalytic performance of a completely saturated Metal Organic Framework, V-MIL-47 [1], for the oxidation of cyclohexene [2]. Furthermore the influence of the amine and nitro functionalized MIL-47 on the epoxidation performance for cyclohexene will be discussed theoretically and experimentally. These new MIL-47 analogues with extra electron donating or withdrawing groups will be compared to the conventional MIL-47 for the oxidation of cyclohexene. Moreover a catalytic cycle, based on molecular modeling of the non-substituted V-MIL-47 will be presented. Also, the effect of substituents on radical generation regeneration of the catalyst will be discussed. All results were modeled on an extended cluster model of MIL-47 on the B3LYP/6-311+g(3df,2p)-D3 level of theory.

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[2] Leus K., Muylaert I., Vandichel M., Marin G. B., Waroquier M.,Van Speybroeck V., Van Der Voort P., Chem.Commun 46 (2010) 5085.