

## Molecular modeling of enantioselective catalysis in chiral MOFs

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Metal organic frameworks (MOFs) or coordination polymers have been a popular topic in research the last three decades. Especially their mesoporous character has led to interesting applications, for example adsorption and gas storage. Recently, they have also been applied as heterogeneous catalysts [1]. The active metal site can be present in many different ways, either within the metal building blocks or incorporated in the linker during a post modification process.

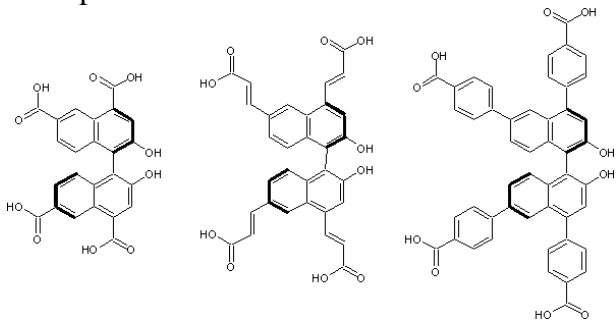


Figure 1: Various (R)-BINOL linkers

In this study, the latter procedure is chosen to build in Ti into various BINOL-type linkers (Figure 1) for use as Sharpless catalyst. This catalyst is currently used in many enantioselective epoxidation processes for allylic alcohols[2]. BINOL linkers have already been incorporated in chiral MOFs by Lin et al.[3]. The feasibility of using this modification for the enantioselective epoxidation is verified by molecular modelling. Hereby, a QM/MM oniom methodology is applied to evaluate the enantioselectivity of the 2,4-pentadien-1-olepoxidation (Figure 2) within the surroundings of the catalyst. Initial calculations on the linker gave an enantiomeric excess of more than 95%. These initial results show the feasibility for using chiral MOFs as heterogeneous catalysts.

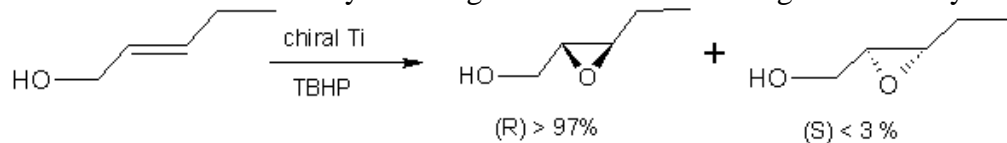


Figure 2: Enantioselective epoxidation with tert-butylhydroperoxide (TBHP)

- [1] Corma A., Garcia H., Xamena F. X. L., Chemical Reviews, 110(2010), 4606.
- [2] Riera A., Moreno M., Molecules, 15 (2010), 1041.
- [3] Lin W. B., Topics in Catalysis, 53(2010), 869.

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