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Poster abstract

WP n°: PL3

Title: The influence of immobilization on the selectivity of Jacobsen-salen complexes

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Summary (max 200 words):

In the last decades salen complexes have proven their value as chiral epoxidation catalysts ¹. Especially with the use of unfunctionalized olefins as a substrate impressive results were obtained. However for a large-scale application, some type of immobilization procedure has to be developed to graft the active complex on a solid support. Previous attempts led to a significant decrease in selectivity. In order to design an immobilization procedure a molecular modeling study was done to unravel the underlying mechanisms for selectivity. This was done by isolating the transition states leading to the various enantiomers with the use of a model that encapsulates the complete system, thus including all steric effects. From these results our models can assess the influence of different immobilization procedures on the catalyst selectivity. This information allows for the design of a procedure where the catalyst is immobilized in the pores of a metal organic framework without the loss of selectivity.

(1) Katsuki, T. *Coord. Chem. Rev.* **1995**, *140*, 189.