

Design of enantioselective catalysts in MOF architectures: a combined theoretical and experimental approach

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In the last decades salen complexes have proven their value as chiral epoxidation catalysts.^[1] The original manganese-salen complex allows the enantioselective epoxidation of unfunctionalized olefins with an enantiomeric excess of over 90%.^[2] To improve the applicability of this catalyst, a heterogenization method is proposed where the homogeneous catalyst is trapped inside the cages of a nanoporous material. As carrier material MIL-101^[3] is chosen, this metal organic framework (MOF) is known for its high internal surface area and large cavities. The encapsulation is performed by introducing the building blocks of the salen ligand in the pores first, allowing them to react to the salen ligand and finally introducing the chelating metal ion. Infrared and elemental analysis results after the first step show the encapsulation of the linker was successful.

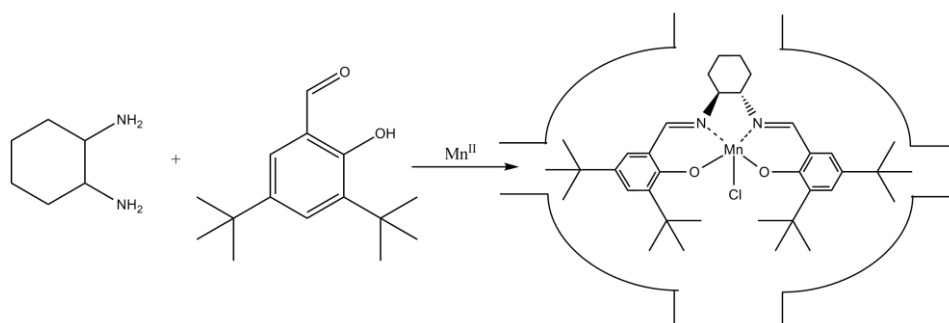


Figure 1: Schematic representation of the encapsulation procedure

Molecular modeling techniques are used to find the detailed reaction mechanism of the salen epoxidation. This gives access to the dimensions needed to accommodate the reaction with different substrates, and will lead to possible modifications to the salen complex to achieve the optimal size. Computational techniques can also provide insight on host-guest interactions that change the behavior of the encapsulated salen complex in catalysis. With this combination of experiments and theory a heterogeneous catalyst that offers the same selectivity as the homogeneous counterpart is designed.

References

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