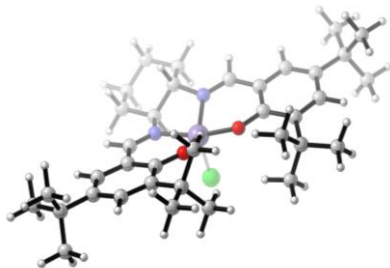Thesisonderwerp 2012-2013 / **MM_12_NANO_16**

MECHANISTIC INVESTIGATION OF AN ENANTIOSELECTIVE CATALYST AS A FIRST STEP IN THE DESIGN OF A HETEROGENEOUS ANALOGUE

Keywords: Mesoporous Materials, chemical kinetics, enantioselective catalysis

Figure 1: Salen catalyst

The metallo-salen complex is a well-known homogeneous catalyst that was originally designed for the enantioselective epoxidation of unfunctionalized olefins. It was the first catalyst that could achieve this efficiently. Besides this epoxidation reaction, the salen complex also proved to be useful in the enantioselective oxidation of sulfides. The goal of this project is to use molecular modeling techniques to gain insight in the mechanism of this reaction. The current computational resources make it possible to design models that take into account various steric interactions that are expected to be important in the selectivity. Another interesting question is the role of the metal center and the counter ion in the complex. Computational techniques are ideal to screen a large amount of metals and ions and find the most active and/or selective one.

Catalyst   *Sulfoxidation reaction*
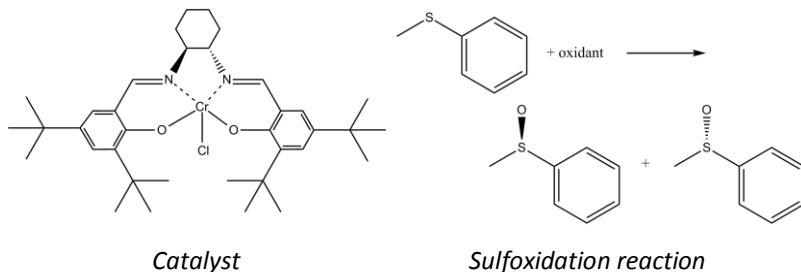
These mechanistic insights can then be used in the design of a heterogeneous analogue for the salen complex. To achieve this we will try to encapsulate the complex in the pores of a metal organic framework. The advantage of this method, better known as a ship-in-a-bottle synthesis, is that the properties of the homogeneous catalyst are directly transferred to the solid material. This allows the combination of the advantages of a heterogeneous catalyst with the well-known behavior of the original complex. Depending on the interest of the student these experiments can be an integral part of the master thesis.

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