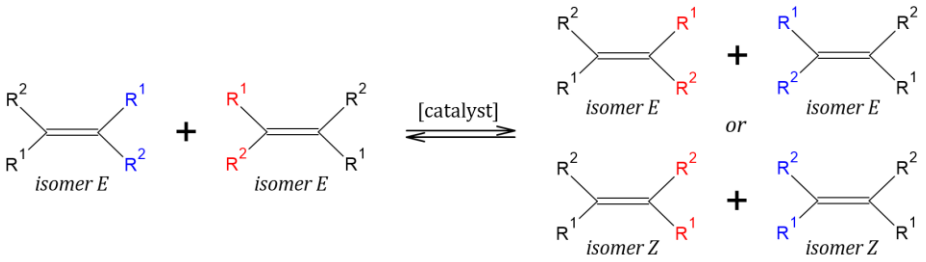
Sustainable Ethenolysis of Renewable Seed Oils with Novel Ruthenium-Based Catalysts

Metathesis, originating from the Greek words for a 'change of position,' is a captivating concept in chemistry. Metathesis can be seen as a molecular rearrangement, in which specific components in organic compounds, such as olefins featuring double carbon-carbon (C=C) bonds, undergo an exchange of substituents R^n:



This process unveils the dynamic nature of chemical reactions at the molecular level, and offers valuable insights into the intricacies of molecular transformations. In this scenario, ruthenium-based complexes play a key role, acting as potent catalysts for olefin metathesis. This chemical process has proven to be a robust and adaptable tool in organic chemistry, offering scientists the ability to craft a diverse array of compounds. The ongoing exploration for novel applications continues to drive curiosity and innovation among researchers across various disciplines in chemistry. Pioneering investigations were awarded the Nobel Prize to laureates Yves Chauvin (*Institut Français du Pétrole*, France), Robert H. Grubbs (*California Institute of Technology*, USA), and Richard R. Schrock (*Massachusetts Institute of Technology*, USA), for the development of the metathesis method in organic synthesis. Beyond its academic roots, olefin metathesis propels breakthroughs in medicinal drugs, fine chemicals, polymeric materials, among others. It is like a scientific domino effect, where one discovery activates a chain reaction of possibilities across diverse fields.

In recent years, scientists have increasingly sought eco-friendly synthetic methods. A notable approach is olefin metathesis, particularly the ethenolysis of renewable seed oils – a sustainable route to craft high-value chemicals. This technique utilizes biomass, such as plant oils, offering a *green* alternative to conventional crude oil and petrochemical sources. The promise of creating sustainable processes shines through when we synthesize valuable chemicals using olefin metathesis. However, as we make improvements in sustainable ethenolysis to contribute to the global energy transition, challenges emerge, especially in dealing with metathesis reactions to produce fine chemicals from renewable sources. This is where the spotlight turns to the essential need for catalysts that are economical, robust, and recyclable. They are the components that make sure these eco-friendly processes go from ambitious ideas to real-world solutions.

The goal of this project is to design and synthesize new ethenolysis catalysts. The performance of this new class of ethenolysis catalysts will be evaluated by means of computational investigations based on quantum-chemical methods. The objectives of this research proposal are planned to be accomplished by three tasks based on computational investigations: (1) assessment of the catalyst activation of the *in silico* designed Ru complexes, (2) determination of catalyst stability due to chemical decomposition, and (3) evaluation of the performance in catalytic cycles with emphasis on ethenolysis of renewable seed oils. In this regard, the energy barriers limiting the reactions shall be calculated; then, in task (4) the Ru complexes that perform metathesis at lower energy barriers will be synthesized in laboratory conditions to assess their catalytic activity. The overall expected result in this scientific project is the introduction of Ru complexes that efficiently catalyze ethenolysis reactions, which serve as a sustainable solution for the synthesis of specific olefinic compounds that have not been explored to date.