Cyclic triel carbenoids as auxiliary ligands for ruthenium-based olefin metathesis catalysts

Tymoteusz Basak

Rarely do we encounter compounds, which obvoiously break the electron octet rule. And it's not without reason—such substances are often simply unstable and they react with virtually anything, to obtain the stable electron configuration. An example of such compounds are carbenes, which contain a carbon atom with six valence elecrons. Non-stabilized "bare" carbenes are just absurdly unstable. They can be stored in inert gas atmosphere for a short time, but traces of air or humidity cause their instantaneous decomposition. However, there exist carbenes, whose structure causes their strongly enhanced stability—both due to electronic factors, reducing the reactivity of the system, and steric ones, which hinder the access to the reactive center. Particularly stable carbenes can even be stored normally in a bottle.

In this project we will not focus on the carbenes themselves, but rather on so-called carbenoids—their analogs, which instead of a carbon atom contain an atom of a different element. In our case it will be triels, the elements from the 13th group of the periodic table. Even though carbenes have been known and studied for dozens of years, the knowledge about triel carbenoids is still in nappies—and that's what we want to change with this project. Our goal is to learn as much as we can about the properties of the carbenoids and to examine catalytic abilities of their ruthenium complexes—potential olefin metathesis catalysts.

In our studies we will use the accomplishments of quantum chemistry. We will not experiment with chemical compounds, but rather simulate reactions with computer programs. We will mostly use the density functional theory (DFT), which enables a very accurate description of the properties of chemical compounds, combined with relatively low computational cost—in other words, the calculations don't last infinitely long and don't require huge amounts of computer power. Because of this, these methods have successfully been used for modeling the structure of compunds and the paths of chemical reactions. Over the course of this project we are going to use the most modern functionals, which excellently describe both typical organic compounds, and those, which contain also transition metals in their structure (for this project the most important one is ruthenium).

The knowledge collected while working on this project will help us understand the mechanisms of studied reactions and the influence of the structure of carbenoids on their catalytic properties. Hopefully, the catalysts we'll design, the ones with the best properties, will be synthesized and studied experimentally in the future, so that they eventually can be used to form interesting and useful substances, so far inaccessible for the humanity.