Rational design of new catalysts for for the synthesis of functionalized organic compounds by cross-coupling reactions

Palladium-catalyzed formation of carbon-carbon and carbon-heteroatom by crosscoupling reactions represents a great interest. These reactions have changed the face of organic synthesis opening new opportunities in preparation of a range of organic compounds for industrial applications.

Despite high popularity of the cross-coupling reactions, they frequently require expensive catalysts mostly based on palladium compounds. High loading of palladium catalysts (10 mol%) and their limited activity adversely affects the efficiency of these processes. Catalyst cost reduction can be achieved by means of a rational catalyst design using more efficient synthetic routes. Furthermore, increasing of chemical and thermal stability of the catalysts and providing them the solubility in water allows to develop environmentally benign systems suitable for application in modification of biomolecules – a new approach for bioengineering synthesis of unnatural amino acids and proteins.

Recently, palladium complexes with acyclic diaminocarbene ligands have proven themselves as one of the most promising new-generation catalysts. They exhibit excellent catalytic properties and are non-sensitive to the presence of atmospheric oxygen and humidity. Our group is one of the pioneers of the catalytic application of acyclic diaminocarbene compounds, including their use in the previously unexplored systems.

Our studies are dedicated to a rational molecular design of new high-performance catalysts on basis of diaminocarbene complexes of palladium for application in cross-coupling processes. In particular, we have developed the first catalytic system on basis of palladiumdiaminocarbenes for carrying out the Suzuki reaction in an aqueous medium. High catalytic activity of the prepared carbene complexes and their hydrophilicity justify their application for functionalization of peptide and other biomolecules. Aminocarbene catalysts that allow the synthesis of substituted alkynes by Sonogashira reaction at room temperature have also been reported. Finally, we have demonstrated the use of metal-diaminocarbene catalysts for the hydrosilylation of terminal alkyne – process closely related to a cross-coupling. All prepared diaminocarbene derivatives were fully characterized by a combination of several physical and chemical methods, and their chemical and catalytic properties were studied in detail.

In total, our research group have published 13 original works on the abovementioned topic.