Novel Ring-Expanded N-Heterocyclic Carbenes and Their Complexes: Synthesis, Evaluation of Steric, Electronic, and Catalytic Properties

N-Heterocyclic carbene (NHC) ligands have gained great importance in organic chemistry, organometallic chemistry, and catalysis due to their interesting properties. Taking into account the entire range of possibilities for modifying their structure, they are of great interest to many research groups. Changes within the ring, i.e. its size, the presence of atoms/groups with different electronic character, as well as the variety of substituents at nitrogen atoms allow for the desired modifications of the steric and electronic properties, which in turn are of key importance for further applications. These ligands are excellent partners of transition metals, creating stable complexes that are successfully used in many catalytic reactions leading to the formation of new carbon-carbon or carbon-heteroatom bonds. The search for new, highly reactive, and selective catalysts is extremely important, as it allows the use of small amounts of NHC-metal complexes under mild reaction conditions.

The aim of the project is to synthesize new N-heterocyclic carbenes of different ring sizes, as well as their complexes, in order to thoroughly investigate their steric, electronic, and catalytic properties. The ligands planned for synthesis, having asymmetric substituents on nitrogen atoms, will enable the filling of the steric gaps between well-defined and widely used NHCs such as IMes, IPr, and IPent. The obtaining of appropriate transition metal complexes will allow for full characterization and evaluation of the relationship between structure and catalytic activity. In addition, the most effective catalysts will be used in late-stage functionalization of medically important compounds.