Organoboron compounds are of great interest to scientists and various stakeholders due to their wide range of applications. They are used in the synthesis of pharmaceuticals, ceramics, materials with specific properties, and in the field of organic electronics. The high demand for the synthesis of organoboron compounds in a selective manner using various types of catalytic processes result in a growing interest in that matter. Transition-metal complexes remain the dominant catalysts used in hydroboration reactions. It is a most commonly used reaction in the synthesis of organoboron compounds. However, the challenges of costly catalyst recycling, separation of reaction products from the (mostly homogeneous) catalyst, use of toxic organic solvents, and overall sustainability of the process are very important in the modern organoboranes chemistry.

Objectives of the research project

The main objective of the project is fundamental research on the development of new organocatalytic methods for the selective hydroboration of unsaturated C-C bonds (in compounds such as alkynes and 1,3-enynes) with a strong emphasis on the principles of Green Chemistry (sustainable process, efficient catalyst recycling and reuse). This project will address issues still superficially described in the literature for hydroboration reactions occurring without the use of metals as catalysts, i.e., i) proper selection of ionic liquids as organocatalysts; ii) effect of substrate structure on process efficiency; iii) ability to recycle the catalytic system. A significant part of the project involves investigating the use of ionic liquids as effective organocatalysts that facilitate the hydroboration reaction. The project, therefore, aims to undertake efforts to develop, assess and demonstrate catalytic methods for the selective hydroboration of C-C bonds using ionic liquids.

Research within the project

The project will focus on the development of novel organocatalytic systems based on ionic liquids that display activity in the selective hydroboration of unsaturated C-C bonds in compounds such as alkynes and 1,3-enynes. These molecules are difficult to functionalize because of the possibility of the formation of different isomers and products. The first stage of the project involves the synthesis of an active and selective organocatalytic system based on ionic liquids and the optimization of reaction conditions. The second step of the project involves screening a wide range of substrates having isolated or conjugated C=C or C≡C bonds to determine the effect of substrate structure on catalyst activity and reaction regio- and stereoselectivity. An important step in the project is the development of an effective method for recycling the organocatalyst, which will be achieved through a strategy based on extraction with an organic solvent (e.g., *n*-heptane). The development of a stable, active, and selective catalytic system and an efficient method for isolating the product from the reaction mixture is a key step in the advancement of catalytic hydroboration of unsaturated C-C bonds. The last stage in the project is the determination of mechanism behind the ionic liquid catalyzed hydroboration reaction, which will be accomplished by the experimental spectroscopic studies and supported by Density Functional Theory (DFT) calculations. Computational analyses will be performed in collaboration with group of prof. Mu-Hyun Baik from the Korea Advanced Institute of Science and Technology (KAIST) and the Institute for Basic Science (IBS). The elucidated mechanism will facilitate significant contribution to the fundamental understanding of the processes catalyzed by ionic liquids.

Justification of research

The issues addressed in the project, i.e., elimination of transition metal-based catalysts, recycling of the catalyst, simple and efficient isolation of products from the reaction mixture, have become a very important research area of leading scientific institutions and industry. However, methods for the synthesis of organoboron compounds based on an organocatalytic approach or, more generally metal-free, with respect to the principles of green chemistry are practically neglected in the scientific literature. Therefore, the implementation of this task within the framework of the project is well justified and will bring a number of benefits, including a) environmental benefits, such as eliminating the use of volatile and toxic organic solvents and expensive transition metal catalysts, b) economic benefits, such as catalyst recycling and one-step product isolation methods leading to shorter process times, and c) scientific benefits, related to expanding fundamental knowledge and providing new solutions for modern organoboron chemistry. The project unlocks a new approach to hydroboration processes based on far less expensive and more accessible catalysts (ionic liquids) compared to systems based on transition metals. A foundation will be established for further development of the designed systems on a larger scale for a wide range of applications: in organometallic and organic chemistry, materials synthesis, and advanced chemicals.