Title of Project : Molecular Activation Directed toward Straightforward Synthesis

Term of Project : FY2010-2014

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【Purpose of the Research Project】

Organic compounds are comprised of a variety of chemical bonds, and synthetic organic chemists have so far been creating compounds through the activation and reconstruction of limited chemical bonds that are relatively easy to activate. Thus, all of the new materials and fine chemicals which have been designed and synthesized based on these known organic transformations tend to be inefficient, multi-step chemical processes. To enable highly efficient synthesis for improvement of organic chemistry in the 21st century, it is essential to develop novel methods to activate rather stable chemical bonds that have been rarely used. This would streamline the processes of catalytic transformation and minimize waste byproducts. This project intensively promotes the rapid development of epoch-making catalytic molecular transformations through the concerted efforts of researchers who have different backgrounds and expertise.

【Content of the Research Project】

Group A01: Exploration of Novel Bond Activation Methods: Members of Group A01 conduct research on the development of catalytic reactions by focusing on the exploration of novel methods of activating molecular bonds. The most important challenge is to develop efficient utilization of hydrocarbons. This will be realized by developing reactions that involve the activation of ubiquitous C-H and C-C bonds in organic compounds. Other goals include exploration of activation methods for various other unreactive bonds, development of catalytic reactions whose key process is the aforementioned bond activation, and achieving innovative straightforward transformation reactions via efficient activation of small molecules such as CO, CO_2, N_2, O_2, simple alkanes and alkenes.

Group A02: Creation of Novel Reactive Species: This group focuses on creating novel reactive species as the basis for activating unreactive bonds and molecules and achieving straightforward molecular transformation reactions. The group aims to create original reactive species that enable innovative molecular transformations, highly reactive species that enable efficient activation of small molecules, reactive species as advanced models of the active sites of biocatalysts, highly activated reactive species that use solid surfaces, and elaborately designed solid catalysts.

Group A03: Constructing Novel Reaction Fields: This group promotes projects involving the design and construction of new reaction fields that enable novel molecular transformations to be pursued rationally and directly by stabilizing or activating catalytically active species and intermediates. The newly developed reaction fields in this group will provide tools for preparing appropriate substrates with tailored specificity and the ability to control selectivity, for example in asymmetric reactions. The development of novel reaction fields will employ systems such as reasonably designed solid-surface reaction substrates, catalytic systems based on any organic compounds and metal complexes, protein matrices including artificial and native enzymes, and supramolecules which include molecular spaces and solid state porous spaces.

【Expected Research Achievements】

When breakthrough achievements have been obtained, novel developments in molecular activation will serve as a driving force to bring about major paradigm shifts in manufacturing processes and lead to significant advances in related research fields such as pharmaceuticals, agrochemicals, materials and polymer sciences. The creation of novel molecular activation methodology has the potential to bring about substantial reforms and innovations in industrial applications such as synthetic organic chemistry used for drug and fine chemicals and, eventually, in industrial-scale production.

【Key Words】

Straightforward Synthesis: Synthesis utilizing unreactive chemical bonds, such as carbon-hydrogen bonds prior to converting reactive chemical bonds, such as carbon-halogen bonds.

【Homepage Address】

http://www.molecular-activation.jp