【Grant-in-Aid for Specially Promoted Research】

Science and Engineering (Chemistry)

Title of Project : Development of Next-Generation Transformation Involving Molecular Activation as a Key Step

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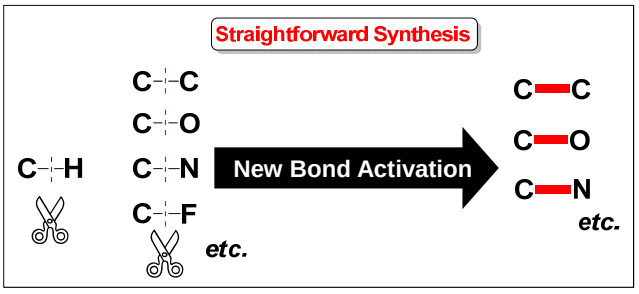
Research Project Number : 17H06091 Researcher Number : 30171953
Research Area : Chemistry
Keyword : Synthetic Chemistry

【Purpose and Background of the Research】

Organic molecules contain a variety of chemical bonds. Organic synthesis involves the cleavage of a chemical bond and the formation of a new one. However, currently, not all of the chemical bonds in organic molecules can be used in organic synthesis. Only reactive and readily available chemical bonds, which are also referred to as functional groups, have been used in organic synthesis. Thus, organic synthesis depends heavily on the reactivity of chemical bonds. To enable highly efficient synthesis for the evolution of organic chemistry in the 21st century, developing novel methodologies for activating rather stable and strong chemical bonds that have been rarely used in organic synthesis, has become an essential aspect in this field of endeavor. This would streamline the processes of catalytic transformation and minimize waste byproducts.

【Research Methods】

One of the typical unreactive bonds is the C-H bond. Although the functionalization of C-H bonds has been extensively studied, some problems that require solutions still remain. Among these are the lack of reaction patterns and the fact that the reactivity and regioselectivity of many reactions cannot be achieved without the use of a directing group. The major focus of this project involves the rapid development of epoch-making catalytic molecular transformations involving new methodologies for the activation of unreactive chemical bonds, such as C-H, C-C, C-O, C-N and C-F, bonds.



Straightforward, Highly Effective, and Safty Synthesis from Simple and Inexpensive Materials Based on Bond Activation

【Expected Research Achievements and Scientific Significance】

If so-called unreactive chemical bonds were to be used directly in organic synthesis, it would provide new possibilities for developing new and straightforward synthetic methodologies based on molecular or bond activation. This would encourage many research groups to participate in this exciting and promising research field, which would permit it to expand and attract more and more attention. The creation of new methodologies would be expected to contribute to a diversity of organic synthesis.

In particular, a new system of C-H functionalization involving the activation of C(sp^3)-H bonds without any specific directing groups, which is the most challenging issue we face today, will be developed.

【Publications Relevant to the Project】

・Nickel-Catalyzed Direct Arylation of C(sp^3)-H Bonds in Aliphatic Amides via Bidentate-Chelation Assistance, Y. Aihara and N. Chatani, *J. Am. Chem. Soc.*, **136** (3), 898-901 (2014).
・M. Tobisu, T. Takahira, T. Morioka, and N. Chatani, Nickel-Catalyzed Alkylative Cross-Coupling of Anisoles with Grignard Reagents via C-O Bond Activation, *J. Am. Chem. Soc.*, **138** (21), 6711-6714 (2016).
・T. Morioka, A. Nishizawa, T. Furukawa, M. Tobisu, and N. Chatani, Nickel-Mediated Decarbonylation of Simple Unstrained Ketones through the Cleavage of Carbon-Carbon Bonds, *J. Am. Chem. Soc.*, **139** (4), 1416-1419 (2017).

【Term of Project】 FY2017-2021

【Budget Allocation】 427,300 Thousand Yen

【Homepage Address and Other Contact Information】

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