【Grant-in-Aid for Specially Promoted Research】

Science and Engineering (Chemistry)

Title of Project : Revolution of Synthetic Technologies by Deeping C-H Activation Chemistry

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Research Area : Organic Synthesis
Keyword : Carbon-Hydrogen Bond Activation, Cross-Coupling, Organic Functional Materials

【Purpose and Background of the Research】

The chemistry of catalytic C-H bond activation has recently been one of the most significant subjects in the area of organic synthesis, as it may lead to new effective molecular transformation reactions. In this research project, we aim at contributing to establish the chemistry field, so that it is applicable to be the truly useful synthetic technology in the development of new organic materials. To this end, the following issues are involved in the research work; (1) development of conceptually new catalytic systems for C-H bond activation and their utilization in challenging molecular transformations such as the functionalization of simple aromatic compounds without bearing any directing group, (2) creation of new functional molecules based on the development of new, practical direct cross-coupling methods, and (3) elucidation of the mechanism of C-H bond functionalization reactions.

【Research Methods】

To accomplish the above objectives, we subject the following research items (1) to (3).

(1) *Development of metal-oxidant cooperative catalysts for direct oxidative coupling of simple aromatic compounds:* The metal-oxidant cooperative catalyst systems are rationally designed by using flexible and multidentate ligands and applied to challenging molecular transformations such as the direct coupling of simple and unfunctionalized aromatic compounds including mother benzene and pyridine skeletons.

(2) *Synthesis and application of novel organic functional materials based on highly condensed planar and non-planar aromatic compounds:* The highly condensed planar and non-planar aromatic compounds are synthesized by using the originally developed catalytic C-H coupling reactions. The planar molecules can be applied to organic semiconductors and organic light-emitting diodes, while circularly polarized luminescence materials are obtained based on the non-planar chiral aromatic compounds.

(3) *Establishment of mechanism of C-H activation through organometallic chemistry, coordination chemistry, and computational chemistry:* Detailed experimental and theoretical mechanistic investigations are carried out, particularly for the clarification of C-H activation mechanism in the catalysis of first- and second-row transition metals such as copper and rhodium. Also, new catalyst systems are designed by the feedback of the mechanistic studies.

【Expected Research Achievements and Scientific Significance】

As described above, this project aims at contributing to create the true value of catalytic C-H bond activation chemistry by developing new catalytic systems for enabling challenging and useful transformations along with elucidation of the reaction mechanisms and their application to the construction of high performance organic materials. Thus, this work may provide new reliable and practical strategies for organic synthesis. It is also expected to contribute to establishment of the sustainable human society through the revolution of chemical synthesis.

【Publications Relevant to the Project】

・Development of Direct Aromatic Coupling Reactions by Transition Metal Catalysis, M. Miura, T. Satoh, K. Hirano, *Bull. Chem. Soc. Jpn.* **2014**, *87,* 751-764.
・Recent Advances in Copper-Mediated Direct Biaryl Coupling, K. Hirano, M. Miura, *Chem. Lett.* **2015**, *44,* 868-873.

【Term of Project】

FY2017-2021

【Budget Allocation】

388,800 Thousand Yen

【Homepage Address and Other Contact Information】

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