【Grant-in-Aid for Scientific Research(S)】
Science and Engineering (Chemistry)

Title of Project : Development of New Methods for Construction of Organic Functional Materials Based on Selective Transformation of Ubiquitous Bonds

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Research Area : Organic Synthesis
Keyword : Activation of Ubiquitous Bonds, Coupling, Organic Functional Materials

【Purpose and Background of the Research】

The activation of ubiquitous bonds such as carbon-hydrogen and carbon-carbon bonds has recently attracted much attention, as it may lead to new, effective transformation reactions, and thus, has been one of the most significant subjects in the area of organic synthesis. The main objective of this research is to design and construct high performance transition metal catalyst systems that allow the selective activation and transformation of the ubiquitous bonds. Based on the new catalyst systems, methods for the effective synthesis of pi-conjugated systems involving an aromatic or heteroaromatic core will be developed. This work may provide new reliable and practical strategies in organic synthesis and afford useful information in developing related areas including coordination chemistry and materials chemistry. It is also expected to contribute to mitigating environmental as well as energy and resource issues.

【Research Methods】

Highly conjugated aromatic and heteroaromatic compounds have recently attracted much attention, as they may exhibit useful physical properties as electronic materials involving semiconducting and luminescent substances. This project aims at developing new synthetic methods for their effective construction based on the selective activation of ubiquitous bonds. The following subjects will mainly be investigated.

(1) Development of high performance catalysts and expansion of substrate applicability: Rational ligand design for the second-row transition metal catalysts involving palladium- and rhodium-based ones is undertaken not only for further enhancing the performance of catalysts for the reactions of aromatic and heteroaromatic substrates which we have developed, but also expanding the substrate scope in our reactions. For ligands, new elaborated cyclopentadienes and nitrogen- or phosphorous-containing ligands are involved. Ligands for bimetallic catalysts are also examined.

(2) Utilization of first-row transition metals: Efficient use of relatively less expensive first-row transition metals as catalysts is undertaken. Reactions that are difficult to achieve even with noble metal catalysts such as dehydrogenative carbon-carbon and carbon-nitrogen couplings are involved as the target transformations.

(3) Development of methods for the construction of new organic functional materials: Based on the new catalytic systems, efficient methods for the construction of pi-conjugated systems having an aromatic or heteroaromatic core are designed, so that they can be potentially useful to prepare the target functional materials.

【Expected Research Achievements and Scientific Significance】

As described above, this project aims at developing new, efficient and practical catalytic reactions for the construction of high performance organic materials having pi-conjugated structures based on the elaboration of transition metal catalyst systems. This work may provide new reliable and practical strategies for organic synthesis based on the selective activation of ubiquitous bonds and afford useful information in related chemistry areas. It is also expected to contribute to sustainable development.

【Publications Relevant to the Project】

- Copper-Mediated Intermolecular Direct Biaryl Coupling, M. Kitahara, N. Umeda, K. Hirano, T. Satoh, M. Miura, *J. Am. Chem. Soc.* **2011**, *133*, 2160-2162.
- Oxidative Coupling of Aromatic Substrates with Alkynes and Alkenes under Rhodium Catalysis, T. Satoh, M. Miura, *Chem. Eur. J.* **2010**, *16*, 11212-11222.

【Term of Project】 FY2012-2016

【Budget Allocation】 167,700 Thousand Yen

【Homepage Address】
http://www.chem.eng.osaka-u.ac.jp/~miura-lab/