【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Chemistry)

Title of Project : Development of Carbon Dioxide Fixation Reactions

Nobuharu Iwasawa
(Tokyo Institute of Technology, Faculty of Science, Professor)

Research Project Number : 17H06143 Researcher Number : 40168563
Research Area : Organic Chemistry
Keyword : Synthetic Organic Chemistry

【Purpose and Background of the Research】

Development of useful methods to utilize carbon dioxide as a one-carbon source is of paramount importance not only from the standpoint of basic science to realize efficient activation of non-reactive molecules, but also from the standpoint of solving the problem of carbon resources facing our society. In this study, based on the research carried out in our group to realize transition metal-catalyzed carbon dioxide fixation reactions, various new approaches will be examined to realize more general and efficient catalytic reactions, and furthermore, conceptually new methods for carbon dioxide fixation reactions will be explored.

【Research Methods】

The basic approach to realize this goal is the development of newly-designed transition metal complexes, which would utilize novel metal-metal interactions to enable efficient catalytic introduction of carbon dioxide into organic molecules. Utilization of solar energy is another important approach, which will also be investigated extensively. For specific examples, various pincer-type complexes containing metal-metal bonds will be prepared for exploration of efficient hydrocarboxylation reactions of unsaturated hydrocarbons and direct C-H carboxylation reactions of various simple hydrocarbons. Novel metallalactone formation and its application to catalytic synthesis of α,β-unsaturated carboxylic acids will also be studied. Combination of photoredox and carboxylation catalysts to realize metallic reductant-free carboxylation reactions and utilization of photo-excited states as reactive species for carboxylation reactions are also important approaches of this research. New methods for activation of carbon dioxide utilizing cooperative interaction between various transition metal complexes will also be investigated.

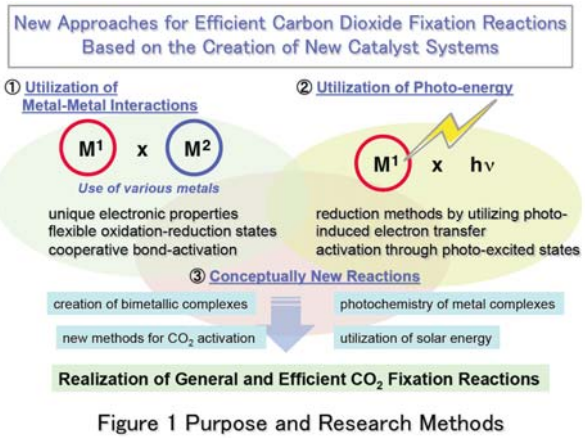

Figure 1 Purpose and Research Methods

【Expected Research Achievements and Scientific Significance】

Development of this research will enable highly useful and efficient atom-economical carbon dioxide fixation reactions, which employ easily available hydrocarbons as starting material. Furthermore, new concepts will be established for novel transition metal catalysis utilizing metal-metal interactions, cooperation of multiple transition metal complexes for developing conceptually new reactions, and utilization of solar energy for CO_2 transformation. This research would also afford new possibilities towards the problem of carbon resources facing our society.

【Publications Relevant to the Project】

・Mechanistic Study of the Rhodium-Catalyzed Carboxylation of Simple Aromatic Compounds with Carbon Dioxide, T. Suga, T. Saitou, J. Takaya and N. Iwasawa, *Chem. Sci.*, **8**, 1454-1462 (2017).

・ Construction of a Visible Light-Driven Hydrocarboxylation Cycle of Alkenes by the Combined Use of Rh(I) and Photoredox Catalysts, K. Murata, N. Numasawa, K. Shimomaki, J. Takaya, N. Iwasawa, *Chem. Commun.,* **53**, 3098-3101 (2017).

【Term of Project】

FY2017-2021

【Budget Allocation】

161,300 Thousand Yen

【Homepage Address and Other Contact Information】

http://www.chemistry.titech.ac.jp/~iwasawa/index.html
niwasawa@chem.titech.ac.jp