

# Science and Technology Group Annual Report FY2021

Satoshi Takebayashi  
Science and Technology Associate

## 1 Introductions

### Project 1: Manganese-catalyzed olefin metathesis

The olefin metathesis reaction is among the most widely applicable catalytic reactions for carbon-carbon double bond formation. Currently, molybdenum- and ruthenium-carbene catalysts are the most common choices for this reaction. It has been anticipated that base metal catalyst would be a desirable economical and biocompatible substitute of the ruthenium-catalysts. *In this project, we are going to develop such base metal catalyzed olefin metathesis reactions using manganese organometallic complexes.*

### Project 2: Direct observation of bond homolysis

Bond homolysis is among the most common bond cleavage mechanisms. Thus, a fundamental understanding of bond homolysis influences the development of a wide range of chemistry. Photolytic bond homolysis and its reverse process have been observed directly using time-resolved spectroscopy. However, direct observation of reversible homolysis remains elusive. *In this project, we are going to develop a system that enables us to directly observe reversible homolysis.*

## 2 Activities and Findings

### Project 1: Manganese-catalyzed olefin metathesis

As a part of this project, I have been investigating the iron-catalyzed olefin metathesis reaction since 2012. This project was accepted in principle by a journal in 2021.

### Project 2: Direct observation of bond homolysis

We investigated the direct observation of reversible Co-Co bond homolysis using two-dimensional nuclear magnetic resonance exchange spectroscopy. The unambiguous characterization of the Co-Co bond homolysis process enabled us to study ligand steric and electronic factors that influence the strength of the Co-Co bond. Understanding of these factors will contribute to rationally designing multimetallic complexes with desired physical property or catalytic activity. Result of this project was presented in the 102<sup>nd</sup> CSJ annual meeting.

## 3 Collaborations

These projects were carried out partly by corroboration with

### Project 1: Manganese-catalyzed olefin metathesis

- Prof. David Milstein (Weizmann Institute of Science)

### Project 2: Direct observation of bond homolysis

- Dr. Robert R. Fayzullin (Arbuzov Institute of Organic and Physical Chemistry, FCR Kazan Scientific Center, Russian Academy of Sciences)

## 4 Publications and other outputs

### Presentation (\*: corresponding presenter)

- (1) Takebayashi, S.\* Fayzullin, R. R., *Isolation of Mononuclear [Co(ligand)(CO)<sub>3</sub>] Metalloradicals and Its H<sub>2</sub> Activation Mechanisms*, Pacifichem 2021, online, December 2021.
- (2) Takebayashi, S.\* Fayzullin, R. R., Bansal, R. *Direct EXSY NMR observation of reversible Co-Co bond*, The 102<sup>nd</sup> CSJ annual meeting, online, March 2022.

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## **5 External fundings**

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<https://kaken.nii.ac.jp/grant/KAKENHI-PROJECT-18K14230/>