May 31, 2022

N.E. CHEMCAT Awarded the Japan Petroleum Institute Award for Encouragement of Research and Development —"Development of NHC-Palladium Complex Catalyst and Immobilized Complex Catalyst by Installation of Silyl Groups on Backbone Carbon"

In the "C-N cross-coupling reaction" used in the synthesis of organic electronic materials and pharmaceuticals, it contributes to reducing the amount of catalyst used and Pd elution and facilitates the filtration process after the reaction.

N.E. CHEMCAT CORPORATION (Head office: Minato-ku, Tokyo; Representative Director & President Matsuru Kushida) is pleased to announced that it was awarded " the Japan Petroleum Institute Award for Encouragement of Research and Development" for the Study on *N*-heterocyclic carbene (NHC)-Palladium Complex Catalysts and Immobilized Complex Catalysts.

In this study, we synthesized a **new *N*-heterocyclic carbene (NHC)-palladium complex catalyst** by direct installation of silyl groups on the backbone carbon of NHC ligands. Specifically, compared to existing NHC-Pd complex catalysts, complex catalysts with dimethylallyl silyl installation **improved catalyst activities by up to 2.5 times**[*1] in C-N cross-coupling reactions, which are used for the synthesis of organic electronic materials and pharmaceuticals. In addition, this complex catalyst can be synthesized in just three steps using commercially available NHC compound as base. It was revealed that the electronic properties of NHC ligands can be converted to electron-donating or electron-withdrawing by changing the substituents on the silicon atom in the silyl group.

In this study, we also successfully synthesized a **immobilized complex catalyst by immobilizing** the NHC-Pd complex catalyst **on polystyrene resin**. The common immobilization method, which uses the substituents attached to nitrogen as binding points, was not able to take full advantage of the bulkiness of NHC ligands, which caused catalytic activities to decline. With this new immobilization method using the silyl groups installed on the backbone carbon as the linking point for the support, the substituents attached to nitrogen of the NHC can be utilized[*1] (Figure 1).

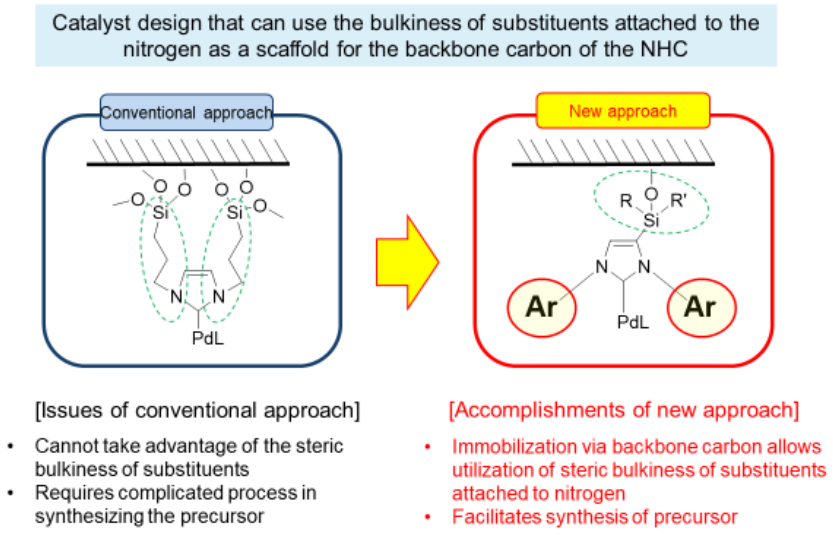

Figure 1. Catalyst design concept

In addition, it was found that, by taking advantage of the improved electronic donating effect, the same level of catalytic activities as NHC-Pd complex can be expressed in C-N cross-coupling reactions. We also achieved significant suppression of residual Pd (<1ppm) after C-N coupling reactions, thereby demonstrating that this is a **unique catalyst having the features of both complex catalyst and immobilization catalyst**[*2] (Figure 2).

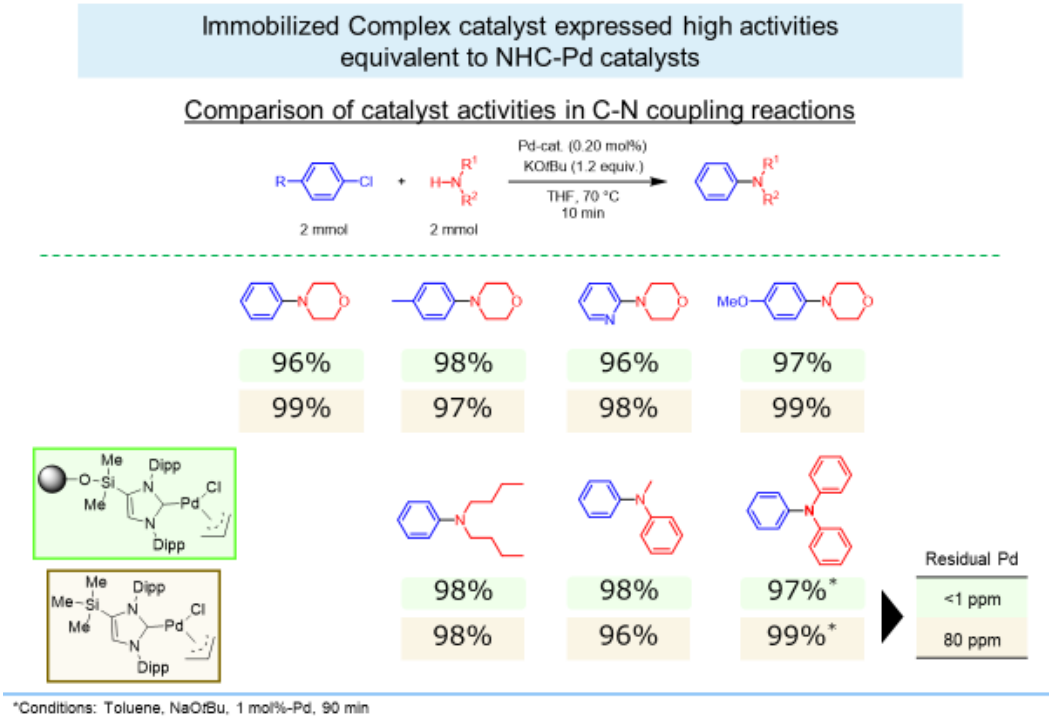

Figure 2. Comparison of catalyst activities of complex immobilization catalysts (Conversion rate of complex immobilization catalyst (above); conversion rates of NHC-Pd complex catalysts (below))

Results were highly appraised from academic and practical perspectives, which led us to win this award.

Going forward, by making these new catalysts available to the industrial sector, N.E. CHEMCAT will contribute to reducing the use of catalysts with improved catalyst activities and simplifying refining process with lower Pd leaching. We will pursue further R&D activities as the catalyst technology that we developed through this study could be applied to catalyst reactions other than C-N cross-coupling reactions and lead to the development of complex immobilization catalysts using metals other than Pd. We are currently setting up for mass production to release these catalysts, and aiming to expand our business even further.

*1 *Organometallics* **2019**, *38*, 375−384. (DOI: 10.1021/acs.organomet.8b00757)
*2 *Organometallics* **2019**, *38*, 1872−1876. (DOI: 10.1021/acs.organomet.9b00159)

∗This research was conducted as joint research between N.E. CHEMCAT Corporation and research groups led by Dr. Jun-Chul Choi, Dr. Norihisa Fukaya, Dr. Kazuhiro Matsumoto, et al. of Catalyst Design Center, National Institute of Advanced Industrial Science and Technology,

- The full explanation on the award can be found on the Japan Petroleum Institute website.

・The Japan Petroleum Institute website: https://www.sekiyu-gakkai.or.jp/jp/aword/2021/210601.html

■ About N.E. CHEMCAT CORPORATION

N.E. CHEMCAT CORPORATION is engaged in the development, manufacturing, and distribution of chemical catalysts, auto exhaust catalysts (including three-way catalysts and diesel auto catalysts), and fuel cell catalysts, and collection/refinement of precious metal catalysts.

[Head Office]	27th floor, World Trade Center Bldg. South Tower, 2-4-1 Hamamatsucho, Minato-ku, Tokyo 105-5127
[Numazu Plant]	678 Ipponmatsu, Numazu City, Shizuoka Pref. 410-0314
[Tsukuba Plant]	25-3 Kohshindaira, Bando City, Ibaraki Pref. 306-0608
[Representative]	Matsuru Kushida, Representative Director & President
[Established]	April 1964
[Capital]	3,423.5 million yen
[URL]	https://www.ne-chemcat.co.jp

■Inquiries on this Release:

N.E. CHEMCAT CORPORATION (Public Relations)
E-mail: info-pr@ne-chemcat.co.jp