New Iron Based Catalysts for C-H Activation

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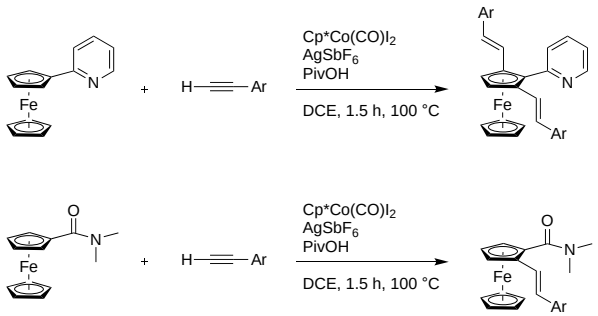
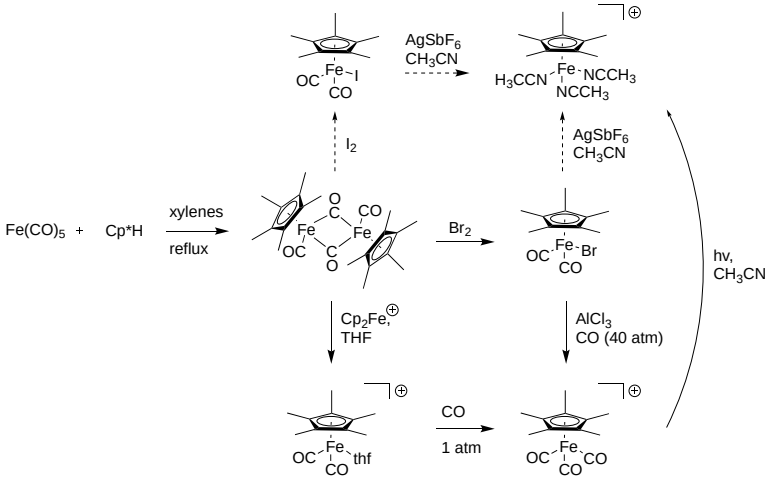
Project Description

Catalytic C-H activation does not need halo or related substituents in order to realize important coupling reactions between aromatic systems and alkyl, alkenyl or alkynyl groups. While such catalytic reactions have been performed by noble metal catalysts (Rh, Ru, Pd…) in the past, we focus on catalytic reactions with less noble, cheaper, and less toxic first row catalysts, namely complexes of cobalt and iron.
The cationic complexes Cp*Co(CO)I2 and Cp*Co(CH3CN)3(SbF6)2 are known to catalyze a variety of C-H functionalization reactions. For example, our group described 2-mono and 2,5-dialkenylations at ODG-bearing ferrocenes (Scheme 1) [1].



***Scheme 1**: Selective di- and monoalkenyla tion at ferrocene using Cp*Co(CO)I2.*

Due to the higher abundance of iron, it could be favorable to substitute the cobalt complexes with iron analogues. The corresponding compounds are literature known (Scheme 2) [2]. However, to our knowledge, they have not yet been used as catalysts in C-H activation reactions. Each of the compounds in Scheme 2 could be a potential precursor for a catalytically active species in C-H activations. Therefore, the synthesis and evaluation of these compounds in reactions such as those in Scheme 1 will be an interesting project for a visiting scientist.



***Scheme 2**: Synthetic routes to Cp*Fe complexes to act as C-H activation catalysts.*

Work developed at LUH

2019	Synthesis of new iron and cobalt catalysts for C-H activation at ferrocene derivatives.
2020	Experiments towards the enantioselective catalytic C-H activation at ferrocene derivatives.
2021	Investigation of interannular stereoinduction at ferrocene derivatives; stereochemistry of catalytic C-H activation at ferrocene.

Work developed at IIT Indore

2019	Investigation of spectroscopic and optoelectronc properties of ferrocene derivatives.
2020	Investigation towards the full characterization of new Cp* iron complexes for catalytic C-H activation at ferrocene derivatives; development of corresponding chiral complexes for enantioselective catalysis.
2021	Application of the new catalysts for the synthesis of compounds of interes for materials chemistry as well as for rug development.

References

1. D. Schmiel, R. Gathy, H. Butenschön, Organometallics 2018, 37, 2095-2110.
2. D. Catheline, D. Astruc, Organometallics 1984, 3, 1094-1100.

Reasoning on Internationalization of Research and Teaching

While the number of international scientists (PhD students, Erasmus fellows, post doc, guest scientists, DAAD and AvH fellows) in the Butenschön group has always been high, the number of scientists from India is still smaller than expected in view of the standard of research in chemistry in India. New Passage to India is therefore a welcome possibility to fil this gap by hosting one or more guest scientists from IIT Indore. As a TU9 university, the links between IIT Indore and TU9 will be strengthened with the option of mutual visits within this scientific cooperation.

Sustainability Factors

Catalysis is the answer of chemistry or the quest of sustainability. Catalytic reactions use new reaction paths requiring less activation energy and resources than conventional reactions and usually take place under comparatively mild reaction conditions.