

論文内容の要旨

論文題目 : **Iron-catalyzed Selective Arylation of C(sp³)-H Bonds**

(鉄触媒を用いた sp³炭素-水素結合の
選択的アリール化反応)

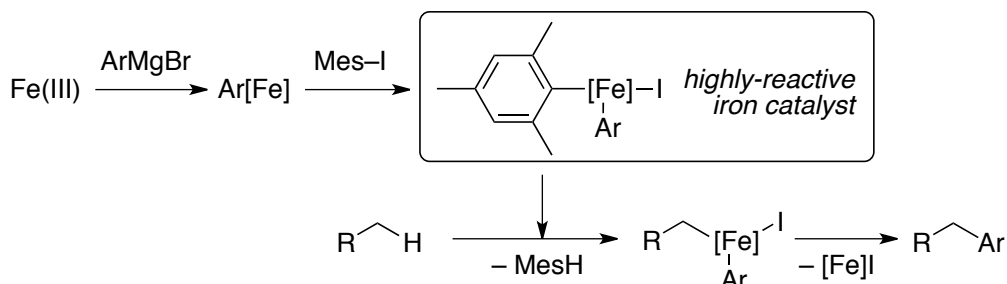
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Organic chemistry has contributed to the development of modern society by providing various bulk and fine chemicals. The realization of a sustainable society requires the invention of more efficient and environmentally benign synthetic methods. The author believes that direct functionalization of C-H bonds and iron catalysis are promising strategies for the chemistry of the next era. The present thesis describes the development of a new reaction model for the iron-catalyzed arylation of a C(sp³)-H bond in simple hydrocarbons.

Chapter 1 describes the motivation of the author. A brief introduction about the significance and challenges in the development of iron catalysis and the difficulties of C(sp³)-H bond functionalization compared to C(sp²)-H bond functionalization are presented.

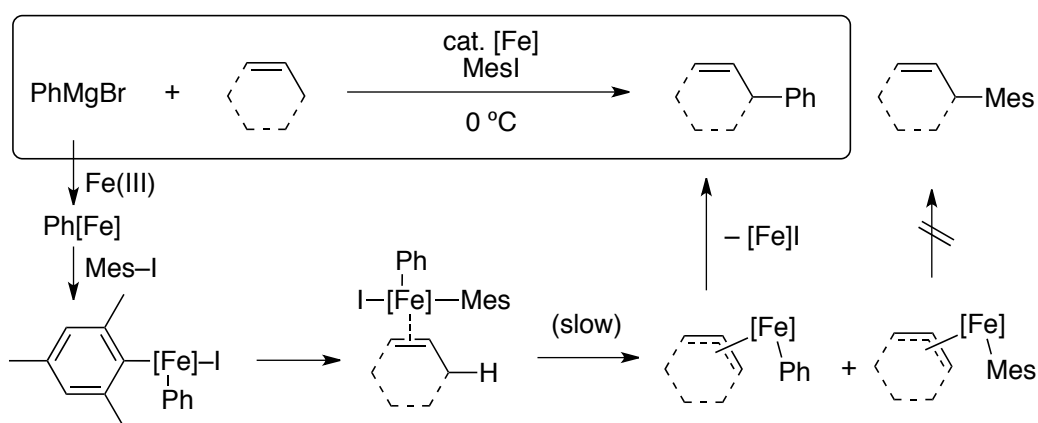
Chapter 2 describes an iron-catalyzed arylation of a C-H bond in saturated hydrocarbons. The synthetic potential of the iron catalytic system was demonstrated for the arylation of an unactivated C(sp³)-H bond (Scheme 1). The regioselectivity of the arylation indicates that the reaction proceeds via homolytic cleavage of the C-H bond by an organometallic iron intermediate.

Scheme 1.



Chapter 3 describes an iron-catalyzed allylic arylation of olefins via C(sp³)-H activation (Scheme 2). By using an aryl Grignard reagent in the presence of bulky aryl iodide, a catalytic amount of an iron salt and a diphosphine ligand, the allylic C-H bond of a cycloalkene or an allylbenzene derivative is successfully converted into a C-C bond under mild conditions. The stereo- and regioselectivity of the reaction, together with deuterium labeling experiments, suggest that C-H bond activation is the slow step in the catalytic cycle preceding the formation of an allyliron intermediate, and that the reductive elimination from the allyliron species is sensitive to sterics.

Scheme 2.



Chapter 4 gives a summary of the thesis, together with perspectives on iron catalysis for C(sp³)-H bond functionalization.