TRANSFER-SEMIHYDROGENATION OF ALKYNES CATALYZED BY AN IRON(II) PCP DICARBONYL ALKYL COMPLEX

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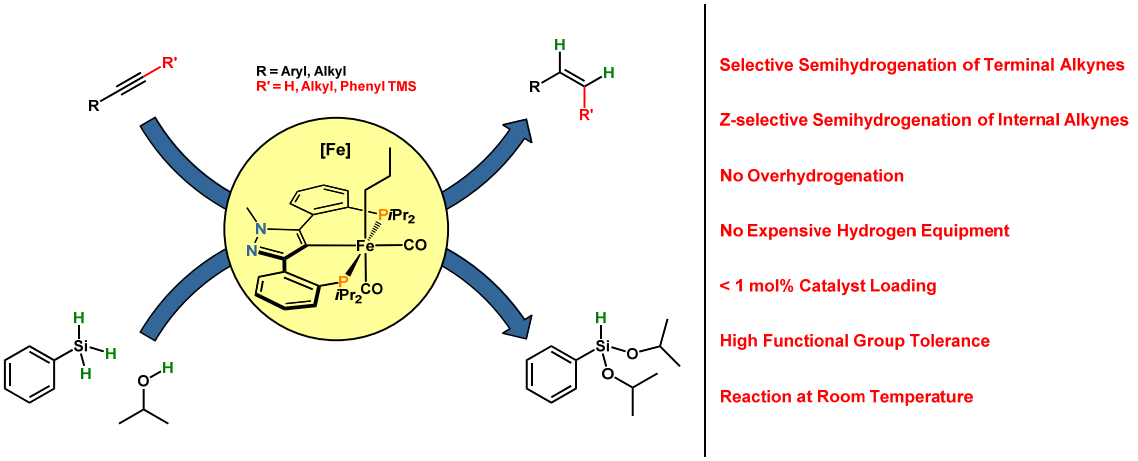
The selective semihydrogenation of alkynes to the respective alkenes is a desirable process in the production of bulk and fine chemicals, pharmaceuticals as well as in research [1]. To avoid the use of special hydrogen equipment, transferhydrogenation processes can be applied. Concerning iron there are rarely transferhydrogenation of C-C triple bonds reported in literature [2-4]

Herein, we report on the transfer-semihydrogenation of terminal and internal alkynes at room temperature catalyzed by a new iron (II) PCP dicarbonyl alkyl complex **[Fe]** comprising an asymmetric pyrazole-derived backbone for the pincer ligand. As hydrogen source a mixture of phenylsilane and 2-propanol is applied (Scheme 1).



Scheme 1. Transfer-Semihydrogenation of alkynes using phenylsilane and 2-propanol catalyzed by an iron (II) PCP dicarbonyl alkyl pincer complex **[Fe]**.

The synthesis, reactivity and characterization of the catalyst **[Fe]** will be discussed in this contribution. Mechanistic aspects of the semihydrogenation will be elucidated by deuteration studies, *in situ* NMR spectra and stoichiometric experiments. These findings are summarized in a derived catalytic cycle, which is further supported by DFT calculations. Additionally, the scope and limitations as well as the selectivity of **[Fe]** for the catalytic semihydrogenation of alkynes will be outlined.

Finally, an outlook towards the functionalization of **[Fe]** to an iron(II) remote NHC dicarbonyl alkyl complex will be given and the catalytic properties of this complex in comparison to **[Fe]** will be discussed.

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