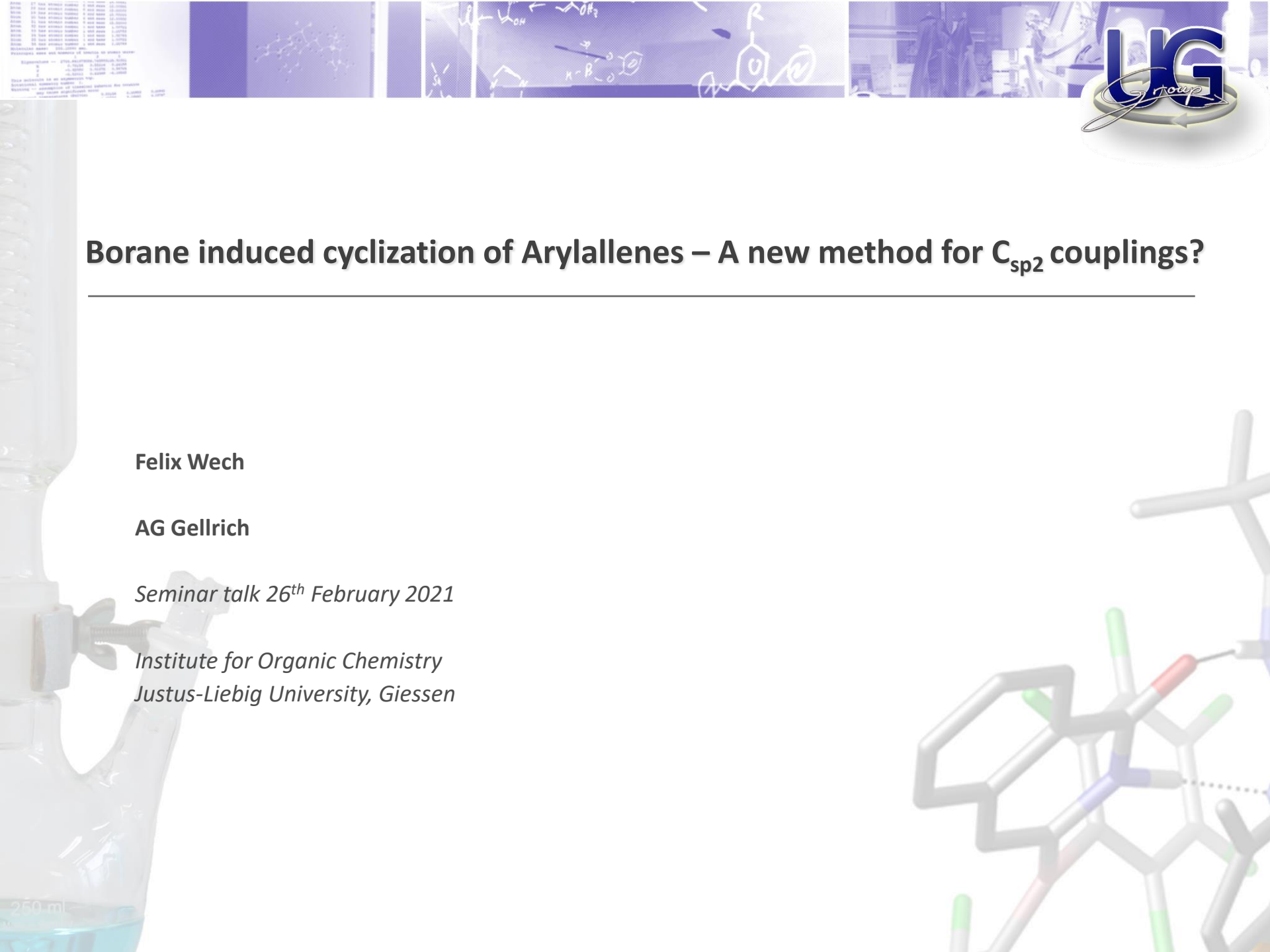




Borane induced cyclization of Aryllallenes – A new method for C_{sp2} couplings?

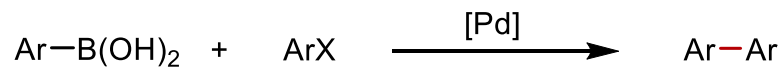
Felix Wech

AG Gellrich

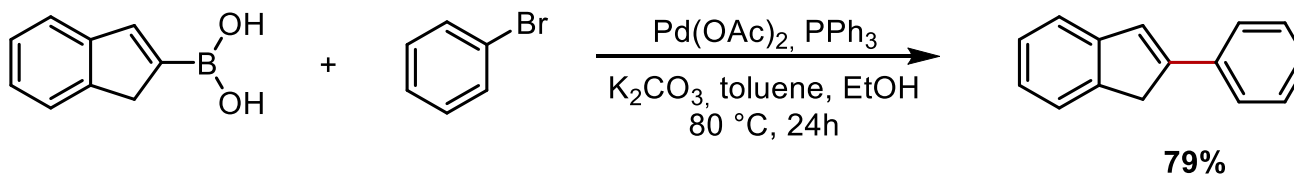
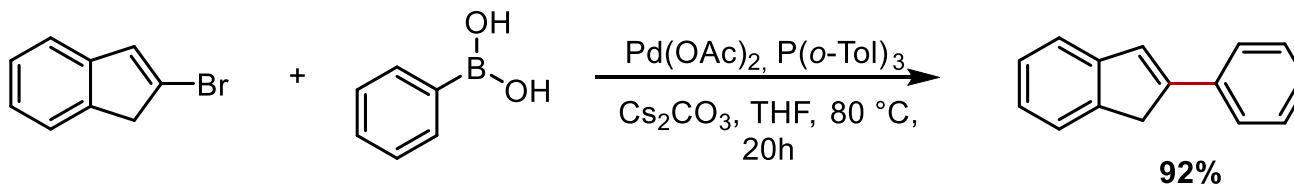
Seminar talk 26th February 2021

*Institute for Organic Chemistry
Justus-Liebig University, Giessen*

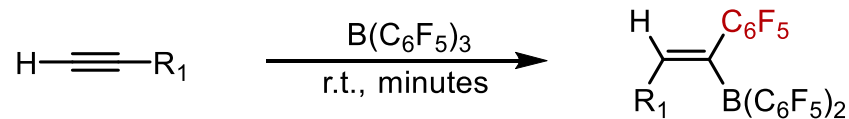
Suzuki-Miyaura Coupling of Indenes



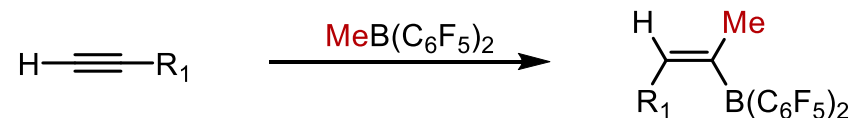
X = Hal



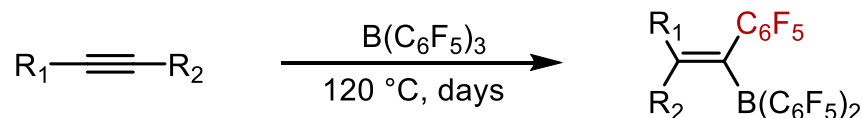
1,1-Carbaborations of Alkynes



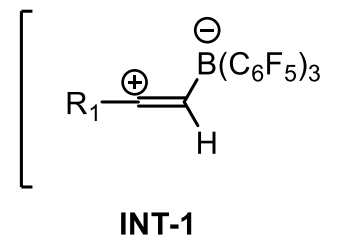
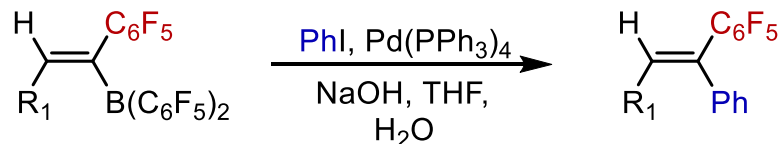
$\text{R}_1 = \text{Ph}, t\text{Bu}, n\text{Pr}$



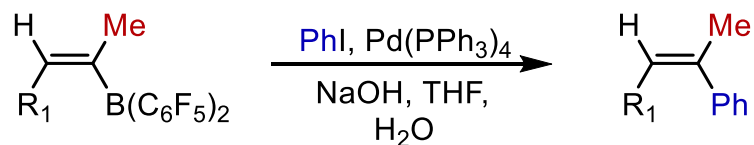
$\text{R}_1 = \text{Ph}, t\text{Bu}, n\text{Pr}$



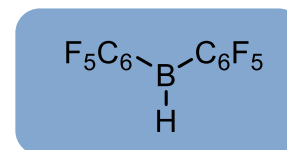
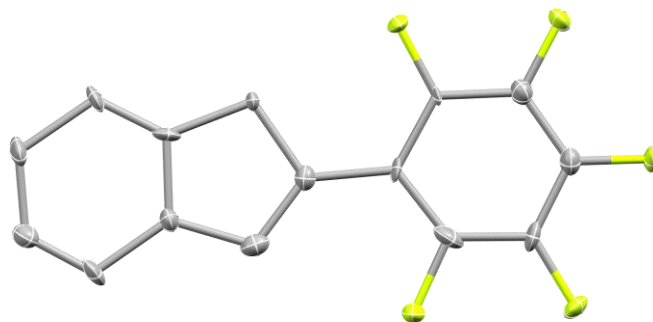
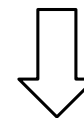
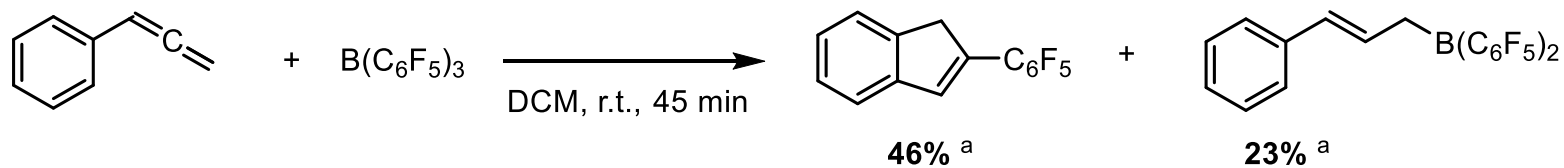
$\text{R}_1 = \text{R}_2 = \text{Ar}$



$\text{R}_1 = \text{Ar}, \text{ferrocene}$

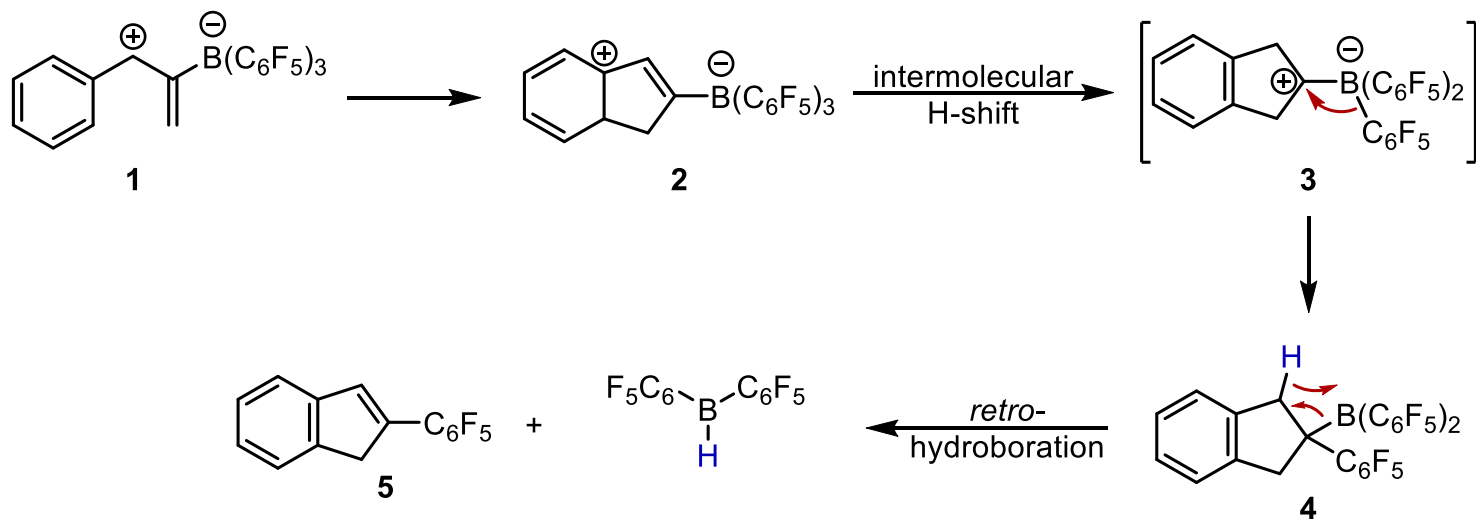
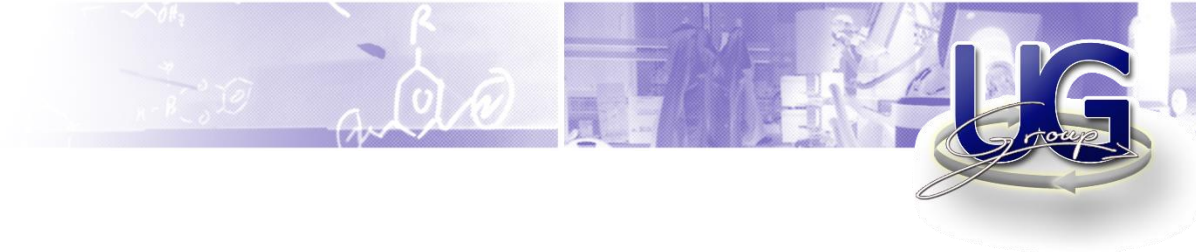


Reaction between $\text{B}(\text{C}_6\text{F}_5)_3$ and Arylallenes

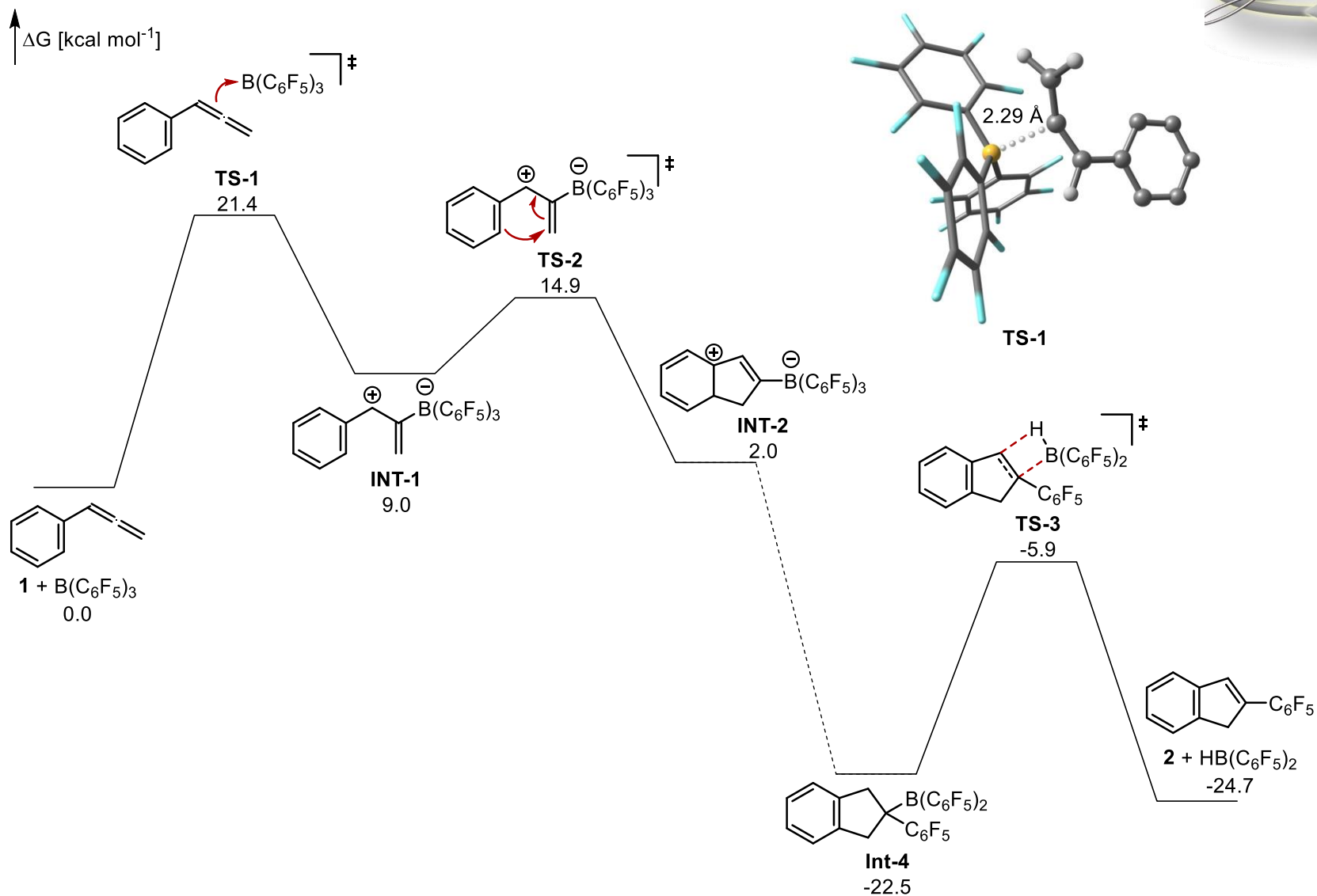


^a yield determined by qNMR using an internal standard.

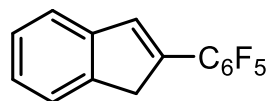
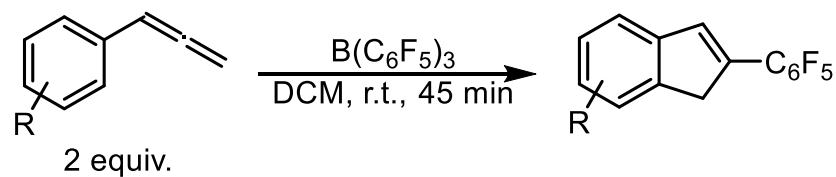
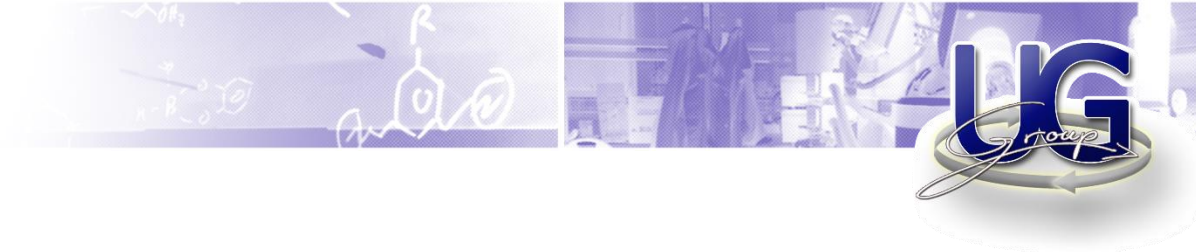
Mechanistic proposal



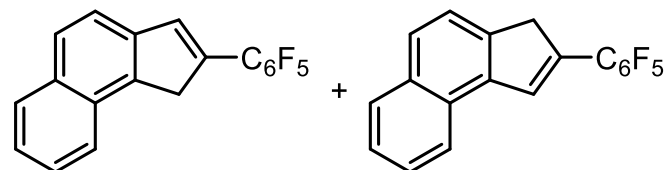
Mechanistic proposal



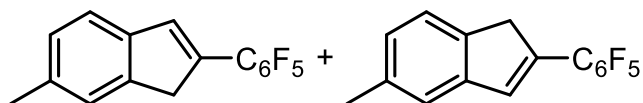
Substrate scope



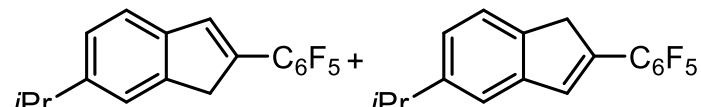
1, 68%



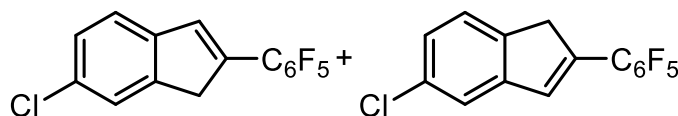
2, 65% (2:1)



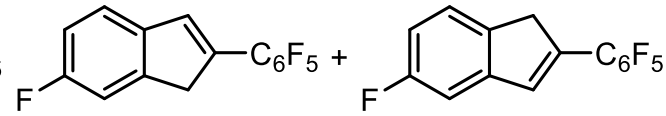
3, 53%^a (2:1)



4, 62%^a (2:1)



5, 45%^b (4:1)



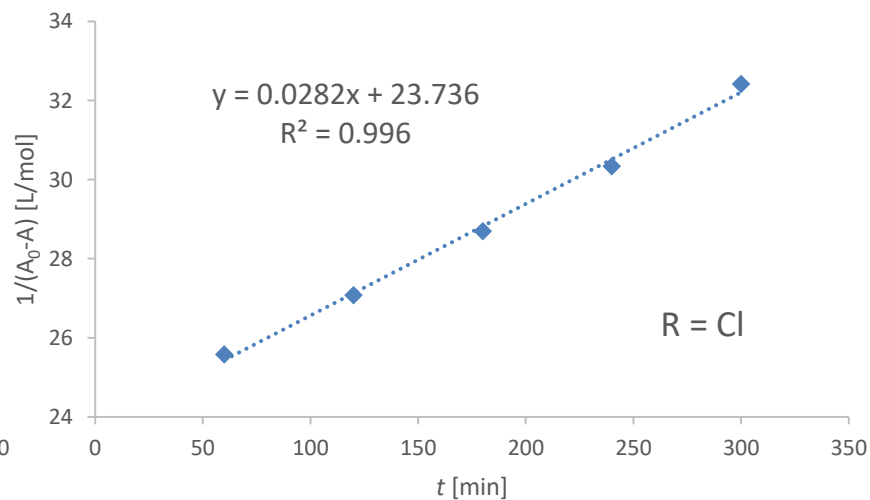
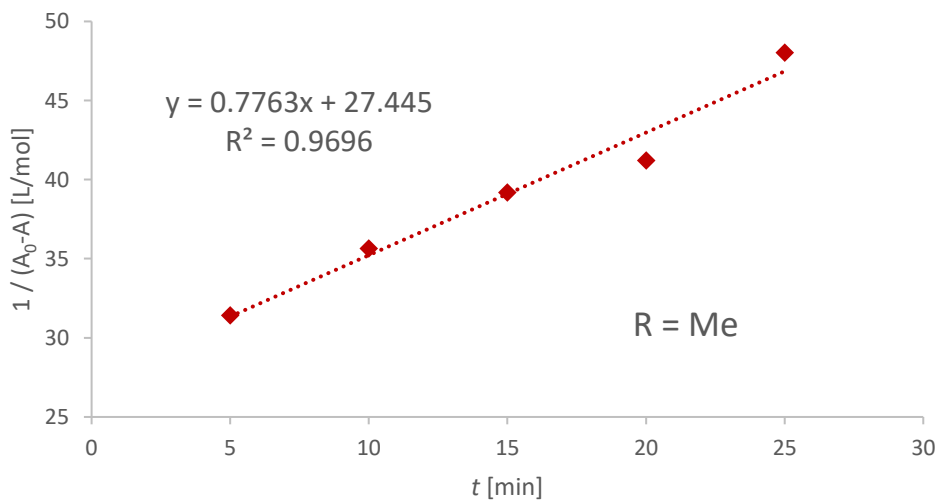
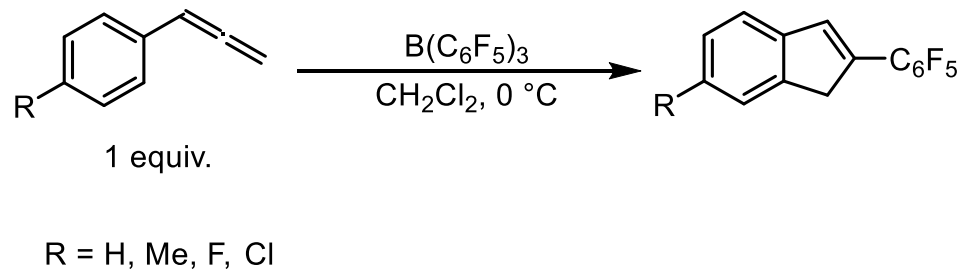
6, 58%^b (4:1)

^a Reaction temperature 0 °C; ^b Reaction temperature 60 °C; isolated yields after column chromatography.

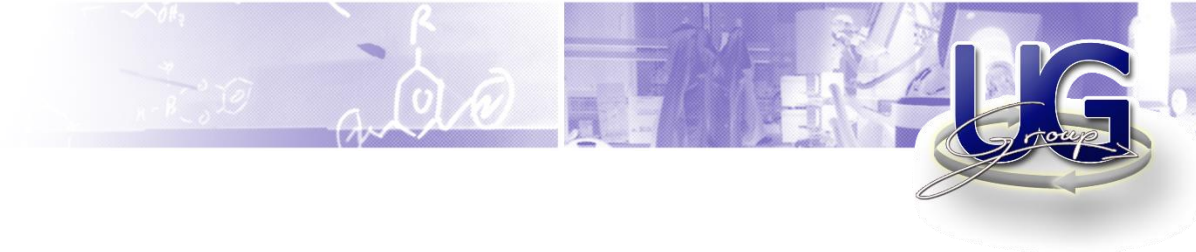
Kinetic measurements



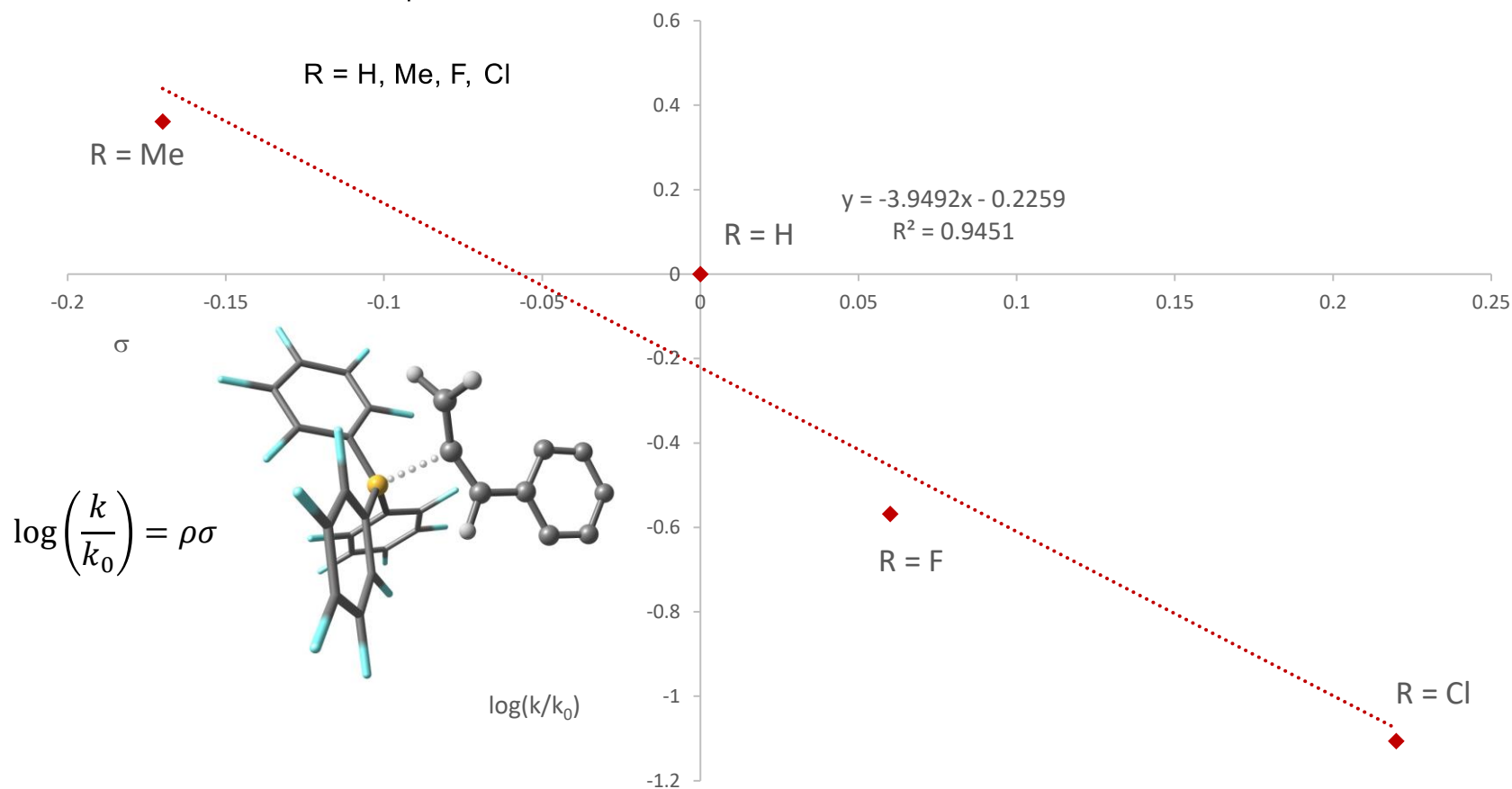
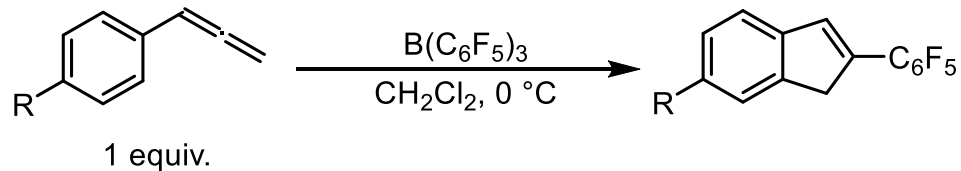
Work in progress



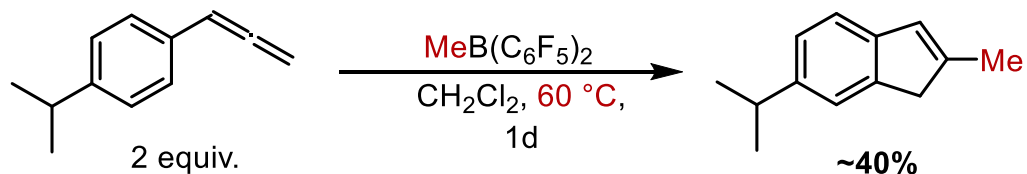
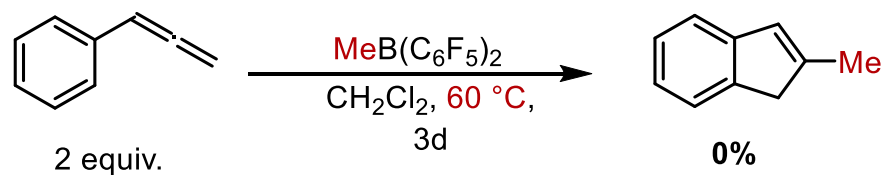
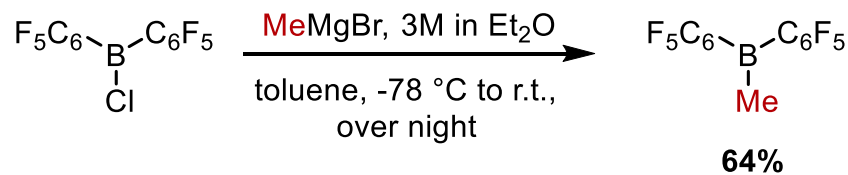
Hammett analysis



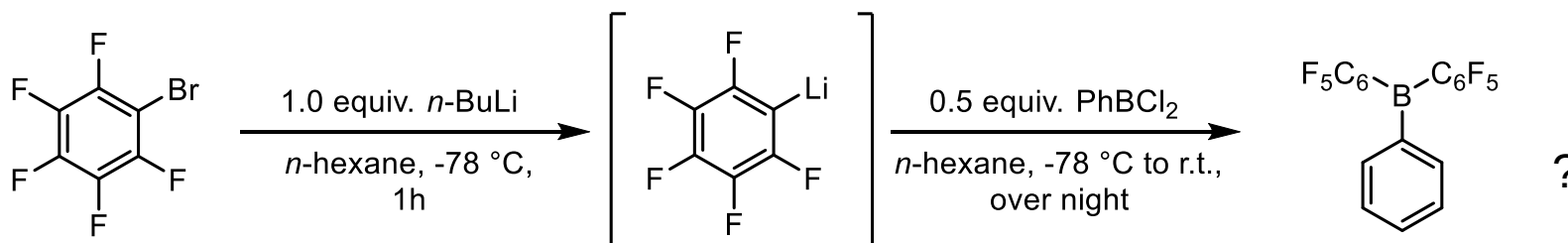
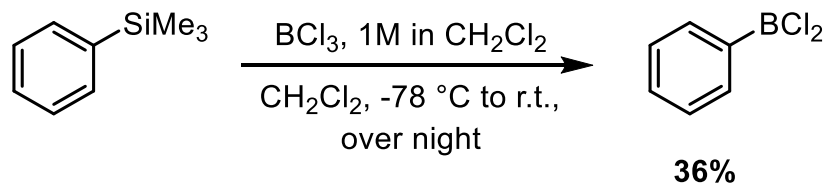
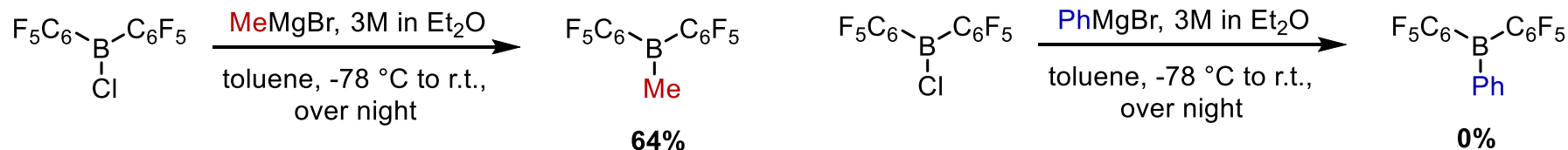
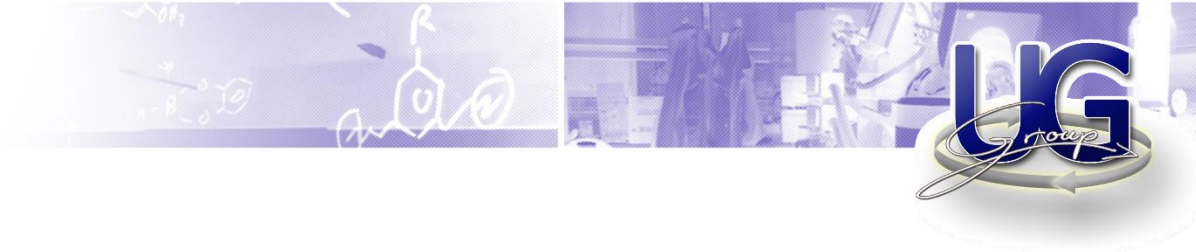
Work in progress



Expanding the scope

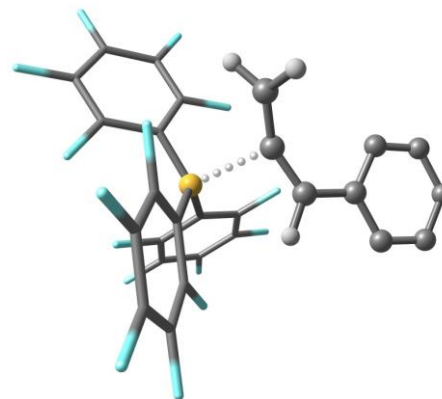
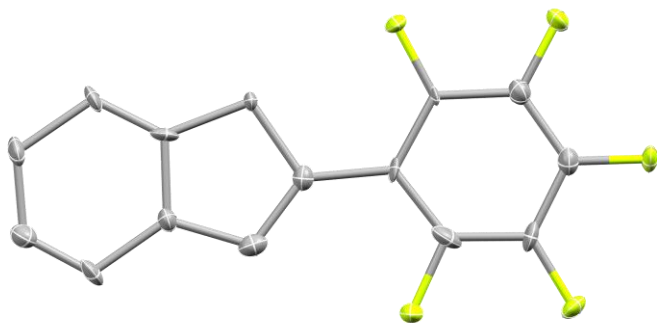


Expanding the scope



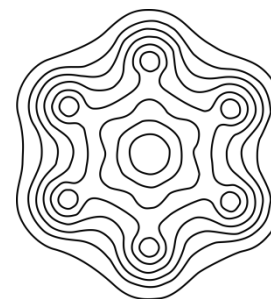


- $\text{B}(\text{C}_6\text{F}_5)_3$ induced cyclization of arylallenes yields C_6F_5 -substituted indenenes
- Computations and kinetics support proposed mechanism
- Focus on the synthesis of new $\text{Ar}-\text{B}(\text{C}_6\text{F}_5)_2$



Acknowledgement

- Dr. Urs Gellrich
- Prof. Dr. Schreiner
- Dr. Hausmann, Dr. Gerbig and the analytics team
- Gellrich Group
- Organic Chemistry Department



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