METAL-LIGAND CATALYZED HETEROCYCLIZATION OF ALLENIC ALCOHOLS

<u>A. Brzozowska</u>,^a J. Sklyaruk,^a L. M. Azofra,^b Y. K. Jang,^a V. Zubar,^a L. Cavallo,^b O. El-Sepelgy,^{a*} M. Rueping^{a,b,*}

 ^a Institute of Organic Chemistry, RWTH Aachen University, Landoltweg 1, 52074 Aachen, Germany
^b KAUST Catalytic Center (KCC), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia aleksandra.brzozowska@rwth-aachen.de

Oxygen-containing heterocycles are present in most naturally occurring and biologically relevant compounds. Therefore, the development of efficient and atom economical methods for the synthesis of these compounds is highly desired.

In my poster I will present the first example of an iron cyclopentadienone complexcatalysed cycloisomerization of substituted allenes leading to the formation of a new carbon–oxygen bond. Notably, readily available allenic alcohols could be smoothly transformed into unsaturated heterocycles, which are important building blocks for the synthesis of bioactive molecules and natural products.^[1,2] Combined experimental and computational studies show that the iron complex exhibits a dual catalytic role in substrate activation, when the non-innocent cyclopentadienone ligand acts as proton shuttle in the isomerization and demetallation steps. Molecular orbital analysis provides insight into that unexpected and selective heterocyclization reaction.



Figure 1. Heterocyclization of Allenic Alcohols.

^[1] El-Sepelgy, O.; Brzozowska, A.; Azofra, L. M.; Jang, Y. K.; Cavallo, L.; Rueping, M. Angew. Chem. Int. Ed. 2017, 56, 14863.

^[2] El-Sepelgy, O. ; Brzozowska, A. ; Sklyaruk, J. ; Jang, Y. K. ; Zubar, V. ; Rueping, M. Org.Lett. 2018, 20, 696.