

Reaction discovery by catalyst design – olefin and N-heterocycle syntheses

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The Kempe Group is interested in homogeneous and heterogeneous catalysis and we call what we do catalyst design. This is to imply that we have an interest in reaction discovery and that our tool to enable a novel chemical reaction is identifying and understanding the right catalyst. We are especially interested in sustainable reaction. In the talk two projects, both are based on molecular or homogeneous catalysts, are discussed namely the *polymerization project* and the *alcohol re-functionalization project*. In the *polymerization project*, we have an interest in selective or on-purpose syntheses of alpha-olefins from ethylene. alpha-Olefins are an important class of chemical compounds and ethylene is an attractive feedstock to synthesize them. However, the selective or on-purpose production of alpha-olefins from ethylene is restricted to three examples, all of them have a linear structure: 1-butene, 1-hexene and 1-octene. We recently discovered an elongation and branching reaction of alpha-olefins by two ethylene molecules [1] and discuss this reaction and its potential for novel selective or on-purpose alpha-olefin syntheses. In the *alcohol re-functionalization project*, we introduced the concept of acceptor-less dehydrogenative condensation for the catalytic synthesis of important aromatic N-heterocyclic compounds. [2] In such reactions, alcohols become selectively hetero-connected via C-C and C-N bond formation steps. The deoxygenation of alcohols takes place via dehydrogenation and condensation steps and H₂ is liberated and can be collected and used if wanted. In the talk, the development of the concept and more recent work, especially a novel mechanism observed for manganese catalysts [3] and accessing novel classes of N-heterocyclic compounds, [4] are discussed.

[1] T. Dietel, F. Lukas, W. P. Kretschmer, R. Kempe, *Science* **2022**, 375, 1021.

[2] S. Michlik, R. Kempe, *Nature Chem.* **2013**, 5, 140.

[3] F. Freitag, T. Irrgang, R. Kempe, *J. Am. Chem. Soc.* **2019**, 141, 11677.

[4] R. Fertig, F. Leowsky-Künstler, T. Irrgang, R. Kempe, *Nature Commun.* **2023**, 14, 595.