

Tangible Chemical Reactions (3-4)

Dipl.-Inf. Univ. Patrick Maier, Prof. Gudrun Klinker, Dr. Markus Drees, Prof. Fritz E. Kühn,

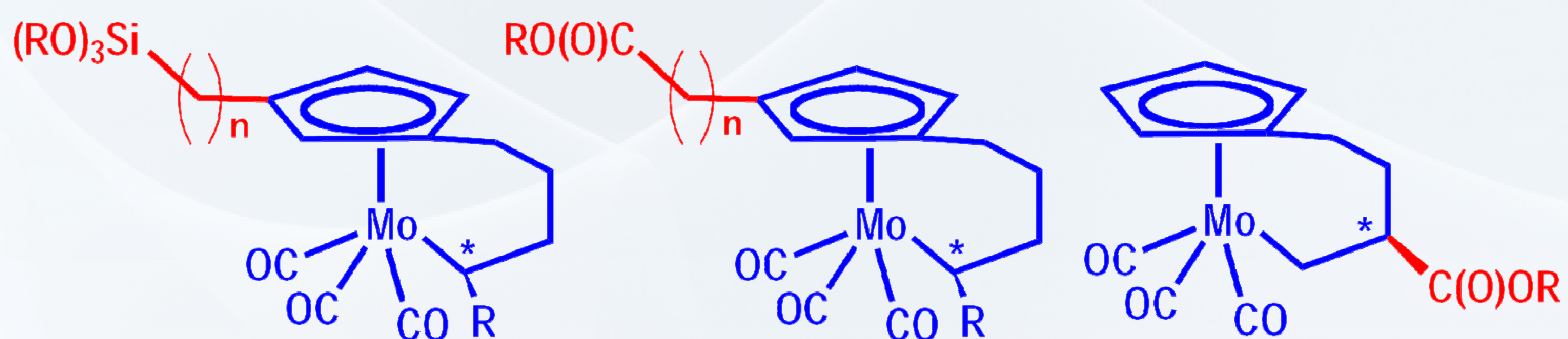
Small Molecules with a Large Impact

Molecular Catalysis

Organomolybdenum complexes of formula $\text{Cp}'\text{MoO}_2\text{X}$ and their precursors $\text{Cp}'\text{Mo}(\text{CO})_3\text{X}$ ($\text{Cp}' = \eta^5\text{-}(\text{C}_5\text{R}_5)$; $\text{X} = \text{Cl}, \text{Br}, \text{CH}_2\text{R}$) are air stable and can be handled in laboratory atmosphere.

The carbonyls need not to be oxidized to the oxides prior to the catalytic reactions, since the oxidizing agent, applied for the catalytic oxidation of the substrates also oxidizes the catalyst precursor to the catalyst in situ.

The molybdenum carbonyl complexes will be both immobilized and attached to chiral ligands in order to enable easy catalyst/product separation and chiral catalysis.



Augmented Chemistry

The augmented reality (AR) group will provide means to visualize the catalyst molecules easily and to understand their dynamic interaction with the substrates. Especially for the chiral catalysis, this will be of utmost importance.

Helping scientists

Of particular importance is the three dimensionality of the computer created molecules and their easy handling and modification, so that laboratory chemists can visualize their intended synthetic goal quickly and get a better idea of the possibility of creating tailor made catalysts.

Advantage

The close contact of laboratory chemists and chemistry students with an informatics research group will help to develop means to understand three dimensional chemical structures much better and faster than with all currently available programs that are usually comparatively difficult to apply and inappropriate for a quick visualization and solution of real laboratory problems.

