Abstract of the Dissertation

Faculty of Mathematics and Natural Sciences at the University of Rostock Doctoral field: Chemistry Titel: "Hydrogenation Reactions Catalyzed by Manganese and Molybdenum Complexes" Author: Niklas Felix Both (E-Mail: <u>niklas.both@catalysis.de</u>) Supervisor: Prof. Dr. Matthias Beller

Hydrogenations represent one of the most important methods for the production of bulk and fine chemicals. Traditionally, homogeneous hydrogenation catalysts are largely based on noble metals such as rhodium, iridium or ruthenium. In light of a growing awareness for more sustainable chemical manufacturing, many scientific approaches focus on the replacement of these metals by non-noble metals due to their economic, ecological and toxicological benefits. Although numerous promising catalysts have been developed, these systems often rely on sophisticated ligands, which limits their practicality. In addition, previous works mainly focused on the transition metals manganese, iron and cobalt, whereas little attention has beenpaid to group 6 metals (chromium, molybdenum and tungsten), despite their equally attractive properties.

In this work, the synthesis of manganese complexes with easily accessible bidentate bis(NHC) ligands and their use as efficient precatalysts for the hydrogenation of carboxylic acid esters as well as ketones, nitriles, N-heteroarenes and alkenes is described. Furthermore, the use of molybdenum catalysts with PNP pincer ligands for the semihydrogenation of alkynes is investigated. Finally, the inexpensive bis(NHC) ligands are used to develop molybdenum-based catalyst systems for the hydrogenation of carboxylic acid esters. The reaction mechanisms of the novel bis(NHC) hydrogenation catalysts were investigated using spectroscopic methods, control experiments and DFT calculations