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Volume Editor

Professor Dr. Gernot Frenking

Philipps-Universität Marburg
Fachbereich Chemie
Lahnberge
35032 Marburg, Germany
frenking@chemie.uni-marburg.de

Editorial Board

Prof. John M. Brown

Dyson Perrins Laboratory
South Parks Road
Oxford OX1 3QY
john.brown@chem.ox.ac.uk

Prof. Alois Fürstner

Max-Planck-Institut für Kohlenforschung
Kaiser-Wilhelm-Platz 1
45470 Mühlheim an der Ruhr, Germany
fuerstner@mpi-muelheim.mpg.de

Prof. Peter Hofmann

Organisch-Chemisches Institut
Universität Heidelberg
Im Neuenheimer Feld 270
69120 Heidelberg, Germany
ph@phindigo.oci.uni-heidelberg.de

Prof. Gerard van Koten

Department of Metal-Mediated Synthesis
Debye Research Institute
Utrecht University
Padualaan 8
3584 CA Utrecht, The Netherlands
vankoten@xray.chem.ruu.nl

Prof. Manfred Reetz

Max-Planck-Institut für Kohlenforschung
Kaiser-Wilhelm-Platz 1
45470 Mülheim an der Ruhr, Germany
reetz@mpi.muelheim.mpg.de

Prof. Pierre H. Dixneuf

Campus de Beaulieu
Université de Rennes 1
Av. du Gl Leclerc
35042 Rennes Cedex, France
Pierre.Dixneuf@univ-rennes1.fr

Prof. Louis S. Hegedus

Department of Chemistry
Colorado State University
Fort Collins, Colorado 80523-1872, USA
hegedus@lamar. colostate.edu

Prof. Paul Knochel

Fachbereich Chemie
Ludwig-Maximilians-Universität
Butenandstr. 5–13
Gebäude F
81377 München, Germany
knoch@cup.uni-muenchen.de

Prof. Shinji Murai

Faculty of Engineering
Department of Applied Chemistry
Osaka University
Yamadaoka 2-1, Suita-shi
Osaka 565, Japan
murai@chem.eng.osaka-u.ac.jp

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Preface

It has been stated in the past that the search for new catalysts has more the character of an art than a science discipline. This is because there was usually more speculation than true knowledge about the reaction mechanisms of catalytic processes. Even the identity of the catalytically active species was frequently not known, which is the reason that systematic testing of all possibly interesting compounds for catalytic reactions was carried out. This is costly and time consuming. The situation has changed in the last decade because much progress has been made in understanding the mechanisms of many catalytic reactions. Besides sophisticated experimental tools, quantum chemical calculations of transition states and reaction intermediates played a prominent role in gaining much better insight into the fundamentals of transition metal catalysis. Estimating solvent effects and the calculation of spectroscopic data are now routinely included in many theoretical studies. Although the design of new catalytically active species is still largely a trial-and-error process, modern research is guided by theoretical calculations in the search for new catalysts, which helps researchers to focus on more promising compounds. The progress in quantum chemical method development has led to the present situation where theory and experiment are synergistically used in an unprecedented manner. In particular, the calculation of transition metal compounds is no longer a too-difficult task for quantum chemistry because efficient methods are available for dealing with many-electron atoms and with relativistic effects.

The seven articles in this volume do not provide a comprehensive view of theoretical investigations of catalytic reactions, because the field has expanded already beyond the scope that can be covered in one book. The contributions written by experts in the field exemplarily demonstrate the strength but also the present limitations of quantum chemical methods for giving insights into the mechanism of transition-metal mediated reactions. Because the development of new theoretical methods is still a very active research area, much progress can be expected in the coming years.

Marburg, Germany, February 2005 Gernot Frenking

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