

Dialkyl Complexes

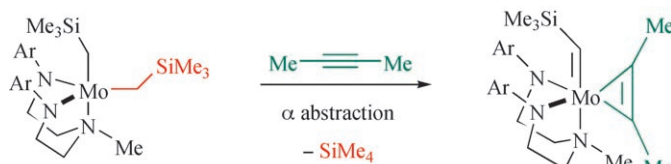
A. S. Hock, R. R. Schrock*

Oxidative Reactions of the Mo^{IV} Dialkyl Complex

$[(3\text{-CF}_3\text{C}_6\text{H}_4\text{NCH}_2\text{CH}_2)_2\text{-NMe}]\text{Mo}(\text{CH}_2\text{SiMe}_3)_2]$

Chem. Asian J.

DOI: 10.1002/asia.200700093



Silicon replacement therapy:

$[(\text{CF}_3\text{N}_2\text{NMe})\text{Mo}(\text{CH}_2\text{SiMe}_3)_2]$ ($(\text{CF}_3\text{N}_2\text{NMe})^{2-} = [(3\text{-CF}_3\text{C}_6\text{H}_4\text{-NCH}_2\text{CH}_2)_2\text{NMe}]^{2-}$) reacts with 2-butyne, cyclohexene sulfide, and C_2Cl_6 to give $[(\text{CF}_3\text{N}_2\text{NMe})\text{Mo}(\text{CHSiMe}_3)(\eta^2\text{-MeC}\equiv\text{CMe})]$, $[(\text{CF}_3\text{N}_2\text{NMe})\text{MoS}_2]$, and $[(\text{CF}_3\text{N}_2\text{NMe})\text{Mo}(\text{CSiMe}_3\text{Cl})_2]$, respectively. $\alpha\text{-H}$ abstraction of Mo^{VI} to yield (initially) $\text{Mo}=\text{CHSiMe}_3$ and SiMe_4 is the proposed route for these reactions.

Biocatalysis

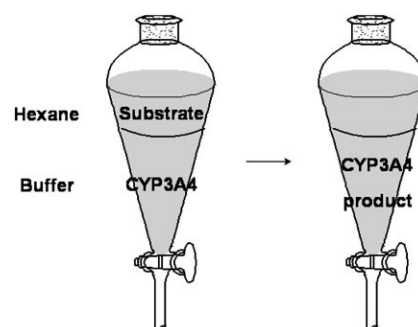
A. Chefson, K. Auclair*

CYP3A4 Activity in the Presence of Organic Cosolvents, Ionic Liquids, or Water-Immiscible Organic Solvents

ChemBioChem

DOI: 10.1002/cbic.200700128

Selective hydroxylation of inactivated C–H bonds. While tolerating only low amounts of water-miscible cosolvents or water-miscible ionic liquids, human CYP3A4 functions acceptably in organic solvents, with optimum activity in buffer/hexane biphasic solvent systems; this offers considerable potential for future applications of P450s in synthesis.



Computational Power

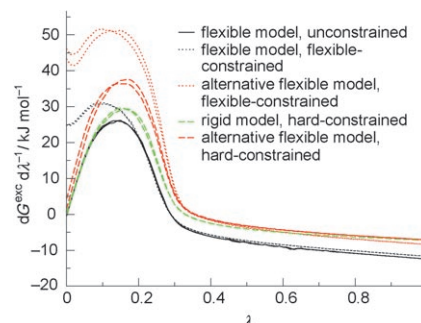
M. Christen, C. D. Christ,
W. F. van Gunsteren*

Free Energy Calculations Using Flexible-Constrained, Hard-Constrained and Non-Constrained Molecular Dynamics Simulations

ChemPhysChem

DOI: 10.1002/cphc.200700176

Turning the water into methanol: One of the most important quantities that can be obtained from simulations are relative free energies. The difference in the free energy of liquid water and liquid methanol is calculated by molecular dynamics simulations using three different models for water and methanol: a flexible model, an alternative flexible model and a rigid model (see picture).



Heterogeneous Catalysis

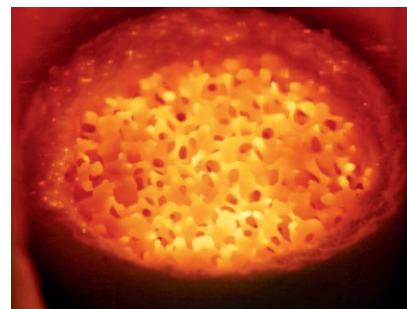
P. J. Dauenhauer, B. J. Dreyer,
N. J. Degenstein, L. D. Schmidt*

Millisecond Reforming of Solid Biomass for Sustainable Fuels

Angew. Chem. Int. Ed.

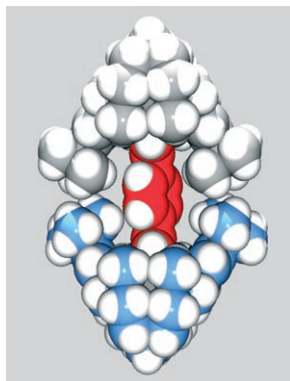
DOI: 10.1002/anie.200701238

Breaking the coke habit: By coupling thermal decomposition with catalytic partial oxidation, an effective method has been developed to convert solid biomass such as cellulose into synthesis gas (see photo of a hot Rh catalyst surface). Not only is the process fast (<70 ms), it also avoids the formation of coke, which is known to deactivate catalyst surface sites and block surface reactions.



Ligand Encapsulation

The ability of 4,4'-bipyrazolate type ligands to link dinuclear LNi_2 units has been examined. The formation of the Ni_4 complexes depends critically on the steric bulkiness of the supporting ligand L and the length of the organic spacer between the connecting heterocycles. The ability of the bipyrazolate moiety to transmit magnetic exchange interactions has also been examined.

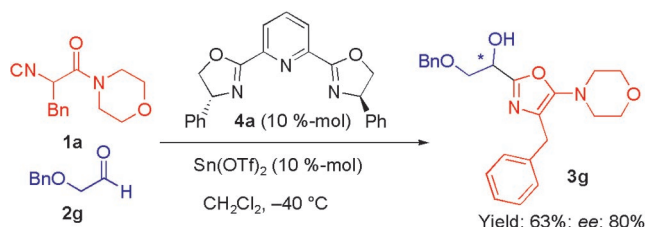


V. Lozan, P. Y. Solntsev, G. Leibeling,
K. V. Domasevitch,* B. Kersting*

**Tetranuclear Nickel Complexes
Composed of Pairs of Dinuclear LNi_2
Fragments Linked by 4,4'-Bipyrazolyl,
1,4-Bis(4'-pyrazolyl)benzene, and
4,4'-Bipyridazine: Synthesis,
Structures, and Magnetic Properties**

Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.200700317

Asymmetric Synthesis



Reactions between α -isocyanoacetamides and aldehydes can be performed at low temperature in the presence of stannous chloride to furnish oxazoles in good to excellent yields. In the presence

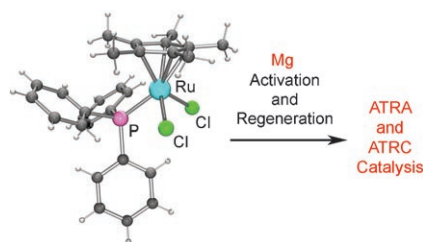
of the chiral catalyst $[\text{Sn}(\text{R})\text{-Ph-PyBox}](\text{OTf})_2$, the reaction between the chelating aldehyde **2g** and **1a** afforded the corresponding 5-aminooxazole **3g** in good yield and enantioselectivity.

S. Wang, M.-X. Wang,* D.-X. Wang,
J. Zhu*

**Asymmetric Lewis Acid Catalyzed
Addition of Isocyanides to Aldehydes
– Synthesis of
5-Amino-2-(1-hydroxyalkyl)oxazoles**

Eur. J. Org. Chem.
DOI: 10.1002/ejoc.200700340

Ruthenium



Radical Reactions: A combined catalyst system of the Ru complex $[\text{RuCl}_2\text{Cp}^*(\text{PPh}_3)]$ (Cp^* : pentamethylcyclopentadienyl) with magnesium allows atom-transfer radical addition (ATRA) and cyclization (ATRC) reactions to be performed with exceptional efficiency under mild conditions (see scheme).

K. Thommes, B. İçli, R. Scopelliti,
K. Severin*

**Atom-Transfer Radical Addition (ATRA)
and Cyclization (ATRC) Reactions
Catalyzed by a Mixture of
 $[\text{RuCl}_2\text{Cp}^*(\text{PPh}_3)]$ and Magnesium**

Chem. Eur. J.
DOI: 10.1002/chem.200700442



On these pages, we feature a selection of the excellent work that has recently been published in our sister journals. If you are reading these pages on a com-

puter, click on any of the items to read the full article. Otherwise please see the DOIs for easy online access through Wiley InterScience.