

## Contents

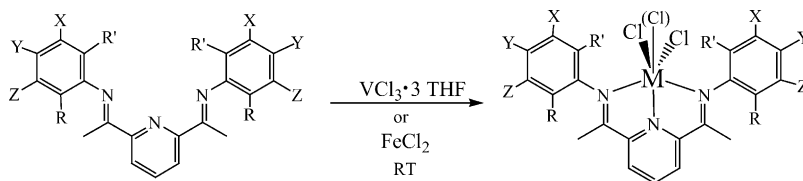
### Articles

**Roland Schmidt, M. Bruce Welch,  
Ronald D. Knudsen, Stefan Gottfried,  
Helmut G. Alt**

*Journal of Molecular Catalysis A: Chemical 222  
(2004) 9*

*N,N,N*-Tridentate iron(II) and vanadium(III) complexes. Part I. Synthesis and characterization

Synthesis and characterization of *N,N,N*-tridentate iron(II) and vanadium(III) complexes.

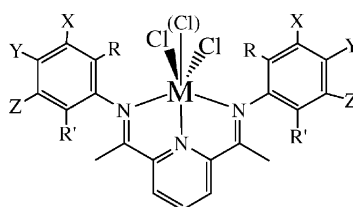


**Roland Schmidt, M. Bruce Welch,  
Ronald D. Knudsen, Stefan Gottfried,  
Helmut G. Alt**

*Journal of Molecular Catalysis A: Chemical 222  
(2004) 17*

*N,N,N*-Tridentate iron(II) and vanadium(III) complexes. Part II: Catalytic behavior for the oligomerization and polymerization of ethene and characterization of the resulting products

Oligomerization and polymerization of ethene with *N,N,N*-tridentate iron(II) and vanadium(III) complexes and characterization of the resulting products.



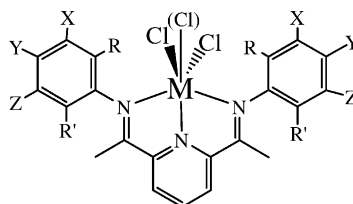
M = Fe(II), V(III)  
R, R' = H, alkyl  
X, Y, Z = H, alkyl, halogen

**Roland Schmidt, Paritosh K. Das,  
M. Bruce Welch, Ronald D. Knudsen**

*Journal of Molecular Catalysis A: Chemical 222  
(2004) 27*

*N,N,N*-Tridentate iron(II) and vanadium(III) complexes. Part III. UV–vis spectroscopic studies of reactions of ethene-oligomerization and polymerization catalysts with methyl aluminoxane cocatalyst

UV-Visible spectroscopic studies on methyl aluminoxane activated *N,N,N*-tridentate iron(II) and vanadium(III) complexes.



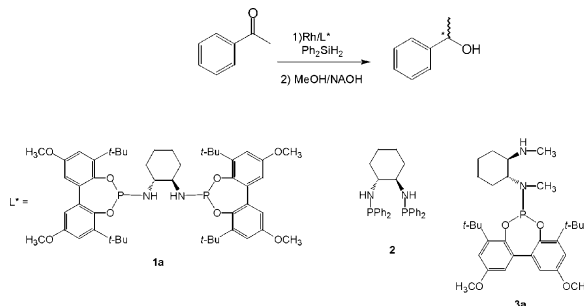
M = Fe(II), V(III)  
R, R' = H, alkyl  
X, Y, Z = H, alkyl, halogen

**Carmela G. Arena, Roberto Pattacini**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 47

Chiral rhodium complexes containing bidentate ligands derived from (*R,R*)-1,2-diaminocyclohexane for catalytic enantioselective hydrosilylation of acetophenone

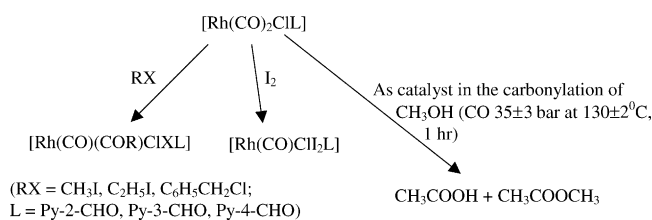
Bidentate P,P- and N,P-ligands derived from the inexpensive and commercially available chiral source (*R,R*)-1,2-diaminocyclohexane, have been tested in the asymmetric Rh-catalyzed addition of diphenylsilane to acetophenone. Studies on the reactivity of these ligands towards the rhodium precursor  $[\text{Rh}(\text{cod})\text{Cl}]_2$  have shown that either monomeric, or dinuclear complexes, or both, can be found in the solution.

**Nandini Kumari, Manab Sharma, Pratap Chutia, Dipak Kumar Dutta**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 53

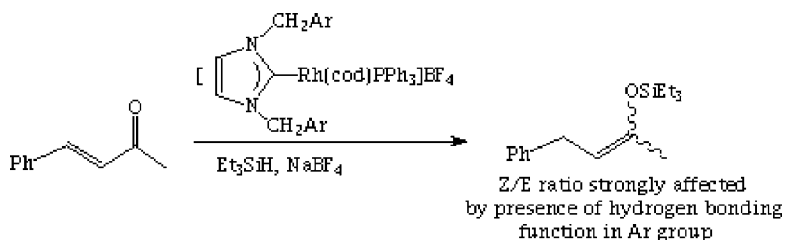
Oxidative addition reaction of rhodium(I) carbonyl complexes of the pyridine-aldehyde ligands and their catalytic activity in carbonylation reaction

Rhodium(I) carbonyl complexes  $[\text{Rh}(\text{CO})_2\text{CIL}]$  ( $\text{L} = \text{Py-2-CHO}$ ,  $\text{Py-3-CHO}$  and  $\text{Py-4-CHO}$ ) have been synthesized and their oxidative reactivity towards different electrophiles like  $\text{CH}_3\text{I}$ ,  $\text{C}_2\text{H}_5\text{I}$ ,  $\text{C}_6\text{H}_5\text{CH}_2\text{Cl}$  and  $\text{I}_2$  were studied. The catalytic activity of the complexes in carbonylation of methanol, in general, is higher than that of the well-known species  $[\text{Rh}(\text{CO})_2\text{I}_2]^-$ .

**Guillermina Rivera, Robert H. Crabtree**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 59

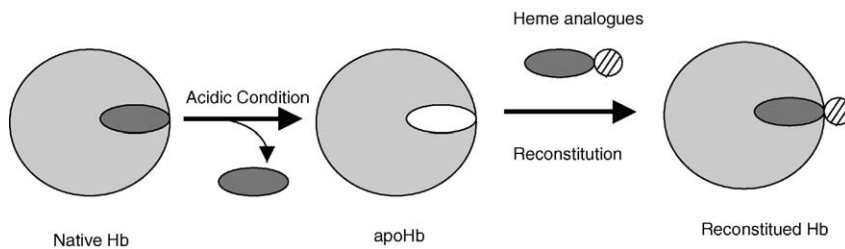
Hydrogen bonding ligand functionality and catalytic selectivity in homogeneous hydrosilylation of enones with rhodium complexes

**Liu Jianyu, Li Yuanzong**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 75

Interaction of apoHb and various Fe-porphyrins

Apo-hemoglobin (apoHb) was reconstituted with heme analogues (FePs). The binding of the FePs on apoHb as well as the peroxidase activities and other properties of the reconstituted Hb were studied.

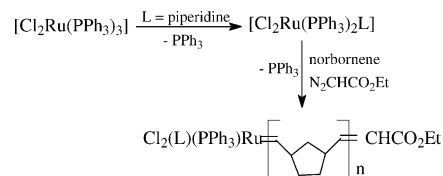


**José Milton E. Matos, Benedito S. Lima-Neto**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 81

Piperidine as ancillary ligand in the novel  $[\text{RuCl}_2(\text{PPh}_3)_2(\text{piperidine})]$  complex for metathesis polymerization of norbornene and norbornadiene

The piperidine behaves as a very good ancillary ligand, enhancing the rate of reaction and controlling the ruthenium metathesis catalysis via a highly active five-coordinated mononuclear Ru(II) complex.

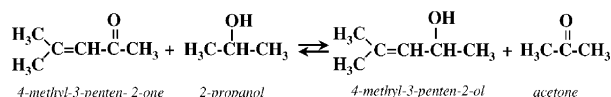


**J.I. Di Cosimo, A. Acosta, C.R. Apesteúa**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 87

Gas-phase hydrogen transfer reduction of  $\alpha,\beta$ -unsaturated ketones on Mg-based catalysts

Gas-phase reduction of 4-methyl-3-penten-2-one (mesityl oxide) to allyl alcohol was studied on basic MgO, Mg–Al and Cu–Mg–Al oxides using 2-propanol as a hydrogen donor. Weak acid–strong base surface pair sites ( $\text{Mg}^{2+}\text{---}\text{O}^{2-}$ ) of MgO promote mesityl oxide adsorption via the C=O bond in a Meerwein–Ponndorf–Verley mechanism preferentially leading to the allyl alcohol.

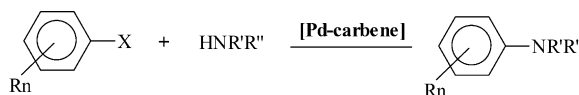


**İsmail Özdemir, Serpil Demir, Yetkin Gök, Engin Çetinkaya, Bekir Çetinkaya**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 97

Synthesis of novel palladium–carbene complexes as efficient catalysts for amination of aryl chlorides in ionic liquid

The synthesis and characterization of  $[\text{PdCl}_2(\text{carbene})_2]$  complexes are reported and their used as catalysts for amination of aryl halides in ionic liquid.

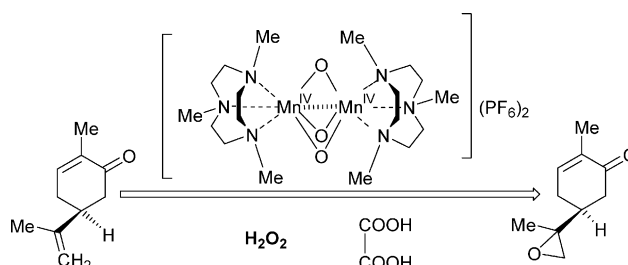


**Camile B. Woitiski, Yuriy N. Kozlov, Dalmo Mandelli, Galina V. Nizova, Ulf Schuchardt, Georgiy B. Shul'pin**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 103

Oxidations by the system “hydrogen peroxide–dinuclear manganese(IV) complex–carboxylic acid”. Part 5. Epoxidation of olefins including natural terpenes

Dinuclear manganese(IV) complex  $[\text{LMn}(\text{O})_3\text{MnL}](\text{PF}_6)_2$  ( $\text{L} = 1,4,7$ -trimethyl-1,4,7-triazacyclononane) efficiently catalyzes epoxidation of sterically accessible olefins, including natural compounds by hydrogen peroxide in acetonitrile at room temperature if a small amount of a carboxylic acid (for example, oxalic acid) is present in the solution.



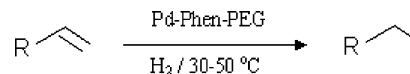


**Unnikrishnan R. Pillai,  
Endalkachew Sahle-Demessie**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 153

Phenanthroline-stabilized palladium nanoparticles in polyethylene glycol—an active and recyclable catalyst system for the selective hydrogenation of olefins using molecular hydrogen

1,10-Phenanthroline-stabilized palladium nanoparticles dispersed in a polyethylene glycol (PEG) matrix is a stable active and recyclable catalyst for the selective hydrogenation of olefins using molecular hydrogen under mild reaction conditions.

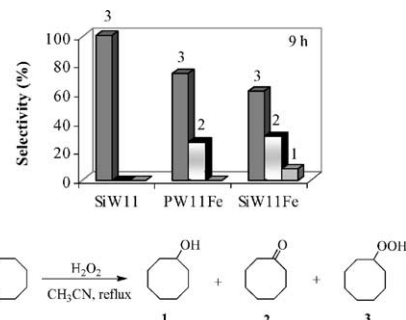


**M. Salet S. Balula, Isabel C.M.S. Santos,  
Mário M.Q. Simões, M. Graça P.M.S. Neves,  
José A.S. Cavaleiro, Ana M.V. Cavaleiro**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 159

A comparative study between Keggin-type tungstophosphates and tungstosilicates in the oxidation of cyclooctane with hydrogen peroxide

Several Keggin-type tungstophosphates and tungstosilicates, including transition metal substituted, lacunary and parent Keggin anions, proved to be active catalysts for the oxidation of cyclooctane with hydrogen peroxide, using acetonitrile as the solvent. Tungstosilicates were less active than tungstophosphates but presented higher selectivity for cyclooctyl hydroperoxide.

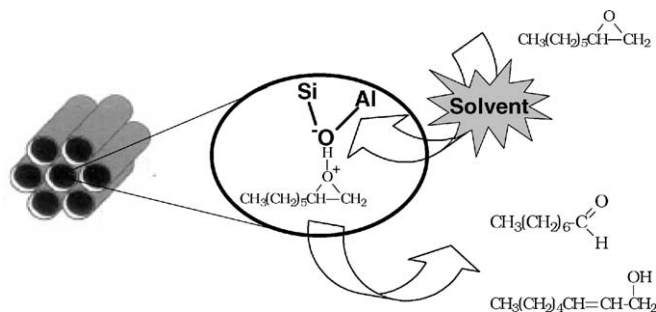


**Rafael van Grieken, David P. Serrano,  
Juan Antonio Melero, Alicia García**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 167

Effect of the solvent in the liquid phase rearrangement of 1,2-epoxyoctane over Al-MCM-41 and Al-TS-1 catalysts

Effect of solvent nature in the catalytic performance of Al-containing zeolitic and mesostructured materials in the liquid phase rearrangement of 1,2-epoxyoctane is reported. The solvent polarity influences strongly on the activity and selectivity.

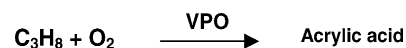


**G. Landi, L. Lisi, J.-C. Volta**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 175

Oxidation of propane to acrylic acid over vanadyl pyrophosphate: modifications of the structural and acid properties during the precursor activation and their relationship with catalytic performances

Evolution of structural and acid properties of VPO during activation under propane–oxygen mixture were studied by XRD, SEM,  $^{31}\text{P}$  NMR,  $\text{NH}_3$ -TPD. Increase of crystallinity, disappearance of  $\text{V}^{5+}$  phases and reduction of acidity are promoted upon water introduction in the activation mixture, selectivity to acrylic acid showing the same trend. Stable catalytic performances and physico-chemical properties are reached after 40 h activation.

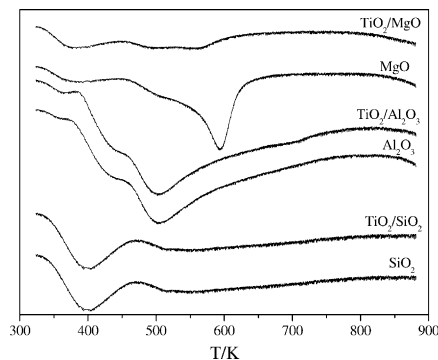


**Xinbin Ma, Shengping Wang, Jinlong Gong, Xia Yang, Genhui Xu**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 183

A comparative study of supported TiO<sub>2</sub> catalysts and activity in ester exchange between dimethyl oxalate and phenol

CO<sub>2</sub>-TPD profile of TiO<sub>2</sub>-supported catalysts. TPD characterization of catalysts accounted for the different total selectivity to MPO and DPO. The weak acid sites were responsible for the formation of MPO and DPO, while the intermediate acid sites and base sites were favorable for the formation of anisole.

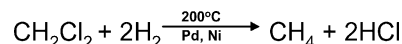


**Beatriz Aristizábal, Carlos Andrés González, Izaskun Barrio, Mario Montes, Consuelo Montes de Correa**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 189

Screening of Pd and Ni supported on sol-gel derived oxides for dichloromethane hydrodechlorination

Xerogel alumina, titania, zirconia and silica modified with Pd and Ni by impregnation and cogelation were examined for the gas phase dichloromethane hydrodechlorination at 200°C. The observed differences in activity are related to the nature and texture of the support and the accessibility of the metal function to the fluid phase.

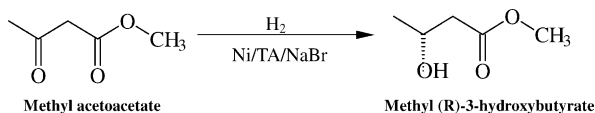


**Donghyun Jo, Jae Sung Lee, Kyung Hee Lee**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 199

Enantio-differentiating hydrogenation of methyl acetoacetate over tartaric acid-modified nickel catalysts: effects of preparation method of supported nickel on activity and selectivity of catalysts

The surface state of nickel has an important effect on the catalysts for the enantio-differentiating hydrogenation of methyl acetoacetate. Unreduced nickel silicate on the catalysts prepared from homogeneous precipitation deposition of nickel on silica constitutes surface defects, thus decreases the enantio-selectivity of catalyst.

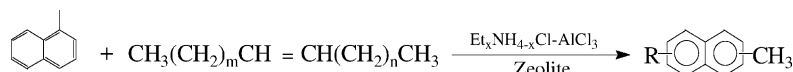


**Zhong-Kui Zhao, Wei-Hong Qiao, Zong-Shi Li, Gui-Ru Wang, Lü-Bo Cheng**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 207

Friedel-Crafts alkylation of  $\alpha$ -methyl-naphthalene in the presence of ionic liquids

Alkylations of  $\alpha$ -methyl-naphthalene with long-chain alkenes (mixed alkenes,  $m + n = 7$  and 8, mass ratio of C<sub>11</sub> to C<sub>12</sub> is 45/55) in the presence of room temperature ionic liquids and zeolite catalysts have been investigated. The Et<sub>x</sub>NH<sub>4-x</sub>Cl-AlCl<sub>3</sub> ( $x = 1, 2, 3$ ) ionic liquids could be an efficient catalyst for long-chain alkylation of  $\alpha$ -methyl-naphthalene.

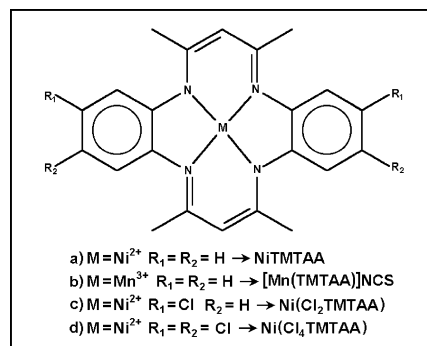


**José Maurício Almeida Caiut,**  
**Shirley Nakagaki,**  
**Geraldo Roberto Friedermann,**  
**Sueli Maria Drechsel,**  
**Aldo José Gorgatti Zarbin**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 213

Nickel(II) and manganese(III) tetraazaannulenes complexes encapsulated in porous Vycor glass (PVG): investigation of catalytic activity

The first immobilization of Ni(II) and Mn(III) metallotetraazaannulene compounds in nanometric pores of an inorganic matrix (porous Vycor glass, PVG) is reported. The catalytic activity of Nickel complex as model of Factor F<sub>430</sub> on the reductive dehalogenation of alkyl halides was studied in homogeneous and heterogeneous systems.

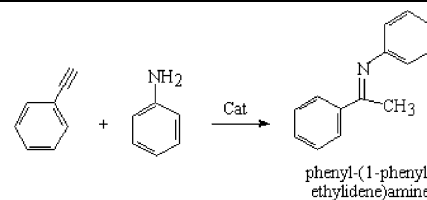


**Ganapati V. Shanbhag, S.B. Halligudi**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 223

Intermolecular hydroamination of alkynes catalyzed by zinc-exchanged montmorillonite clay

Intermolecular hydroamination of phenyl acetylene by aniline to give phenyl-(1-phenylethylidene)amine was investigated using Zn<sup>2+</sup> exchanged K-10 montmorillonite clay. Zn/K-10 and Zn/H-beta showed comparable activity with high regioselectivity.

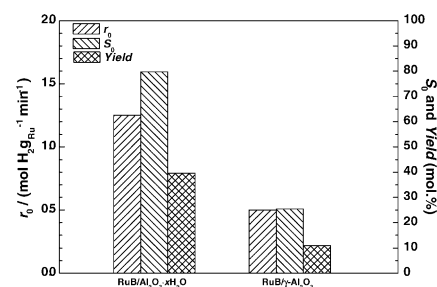


**Jianqiang Wang, Pingjun Guo, Shirun Yan, Minghua Qiao, Hexing Li, Kangnian Fan**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 229

Colloidal RuB/Al<sub>2</sub>O<sub>3</sub>·xH<sub>2</sub>O catalyst for liquid phase hydrogenation of benzene to cyclohexene

A novel colloidal RuB/Al<sub>2</sub>O<sub>3</sub>·xH<sub>2</sub>O catalyst exhibiting superior catalytic performance to the RuB/γ-Al<sub>2</sub>O<sub>3</sub> catalyst in liquid phase selective hydrogenation of benzene was prepared by a combined coprecipitation–crystallization–reduction strategy.

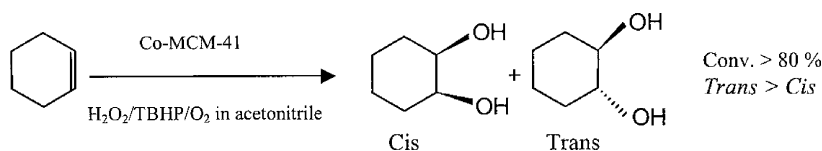


**S. Samanta, S.C. Laha, N.K. Mal, A. Bhaumik**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 235

Co(III)-containing mesoporous silica as an efficient catalyst in selective dihydroxylation of cyclohexene

Novel Co-containing mesoporous material showed excellent activity in the liquid phase selective oxidation of cyclohexene in an environmentally friendly catalytic route with easy product separation and no undesired side product.

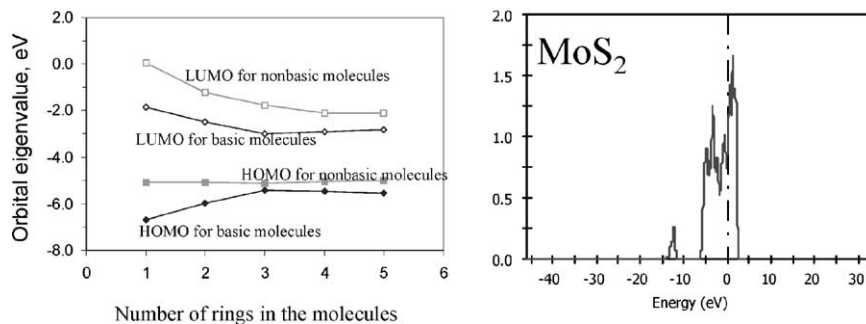


**Mingyong Sun, Alan E. Nelson, John Adjaye**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 243

Correlating the electronic properties and HDN reactivities of organonitrogen compounds: an ab initio DFT study

The HDN reactivities of organonitrogen compounds are correlated to their electronic structures and properties. Adjusting electronic structures of hydrotreating catalysts changes catalyst HDN selectivity for basic and non-basic nitrogen compounds.

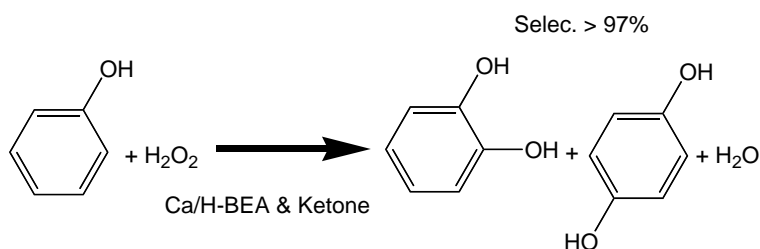


**Takashi Atoguchi, Tomonori Kanougi**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 253

Phenol oxidation over alkaline earth metal ion exchange beta zeolite in the presence of ketone

The oxidation of phenol into catechol and hydroquinone proceeds catalytically in a highly selective manner in the presence of Ca/H-BEA and a small amount of ketone.

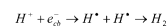
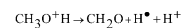
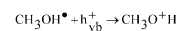
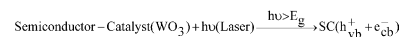
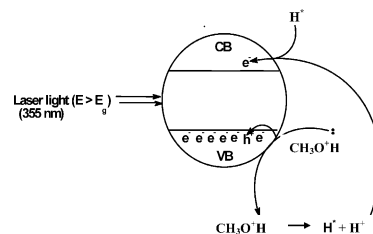


**M.A. Gondal, A. Hameed, Z.H. Yamani**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 259

Hydrogen generation by laser transformation of methanol using n-type  $\text{WO}_3$  semiconductor catalyst

A laser based method for photo-catalytic reforming of methanol into non explosive mixture of gases ( $\text{H}_2$ ,  $\text{CO}_2$  and  $\text{CH}_4$ ) with major part of hydrogen over n-type  $\text{WO}_3$  semiconductor catalyst was carried out. The amount of catalyst and laser energy was optimized for maximum yield of hydrogen.



**Jin Zhao, Ana M. Santos, Eberhardt Herdtweck, Fritz E. Kühn**

*Journal of Molecular Catalysis A: Chemical* 222 (2004) 265

Molybdenum and tungsten complexes of composition  $(\eta^5\text{-C}_5\text{R}_5)\text{MR}'(\text{CO})_3$  and their use as olefin epoxidation catalyst precursors

