



www.elsevier.com/locate/molcata

### Contents

#### **Articles**

### Fan Yang, Lin-Mei He, Hua Yi, Gang Zou, Jie Tang, Ming-Yuan He

Journal of Molecular Catalysis A: Chemical 273 (2007) 1

An efficient silica-grafted poly-(L)-leucine catalyst for asymmetric epoxidation of  $\alpha,\beta$ -unsaturated ketone

A new efficient covalent immobilization method for preparation of silica-grafted poly-(L)-leucine catalyst AP-PLL-Silica gel was developed. The AP-PLL-Silica gel catalyzed asymmetric epoxidation of benzalace-tophenone, yielding optically active epoxy ketone in high enantioselectivity up to 97% e.e. The catalyst was easily separated and reused several times with no significant loss of activity and enantioselectivity.

$$n \text{ (L)-Leu NCA} \xrightarrow{\text{APTESi}} \text{EtO-Si} \xrightarrow{\text{OEt}} \text{H} \xrightarrow{\text{R}} \text{N} \xrightarrow{\text{N}}_{n} \text{H} \xrightarrow{\text{Silica gel}} \text{OEt} \xrightarrow{\text{N}} \text{N} \xrightarrow{\text{N}}_{n} \text{H}$$

$$AP-PLL \qquad \qquad \text{AP-PLL-Silica gel}$$

### Maw-Ling Wang, Venugopal Rajendran

Journal of Molecular Catalysis A: Chemical 273 (2007) 5

Kinetics for dichlorocyclopropanation of 1,7-octadiene under the influence of ultrasound assisted phase-transfer catalysis conditions The synthesis of dichlorocyclopropane derivatives of 1,7-octadiene by quaternary ammonium salts in a liquid—liquid two-phase medium was carried out in the presence of ultrasonic waves. Kinetics of the reaction is investigated in detail.

### Zhen Liu, Li Huang, Wen S. Li, Feng Yang, C.T. Au, Xiao P. Zhou

Journal of Molecular Catalysis A: Chemical 273 (2007) 14

Higher hydrocarbons from methane condensation mediated by HBr

Methane was condensed to higher hydrocarbons by a hydrogen bromide mediated catalytic process. Methane was converted to bromomethanes by reacting with oxygen and HBr over the first catalyst, and then bromomethanes were converted to higher hydrocarbons to regenerate HBr.

$$CH_4+CO$$
 $CO_2$ 
 $CH_4+CO+CO_2$ 
 $CH_4+O_2$ 
 $CH_4+O_2$ 

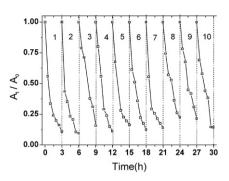
vi Contents

### Jianchun Wang, Ping Liu, Shiming Wang, Wei Han, Xuxu Wang, Xianzhi Fu

Journal of Molecular Catalysis A: Chemical 273 (2007) 21

Nanocrystalline zinc oxide in perfluorinated ionomer membranes: Preparation, characterization, and photocatalytic properties

ZnO nanocatalysts embedded in Nafion membranes exhibited excellent photocatalytic activity and high stability against photocorrosion in the photodegradation of rhodamine B.



#### M. Lakshmi Kantam, Sarabindu Roy, Moumita Roy, Bojja Sreedhar, B.M. Choudary, Rajib Lal De

Journal of Molecular Catalysis A: Chemical 273 (2007) 26

Layered double hydroxides supported rhodium(0): An efficient and reusable catalyst for Heck, Suzuki, and Stille reactions of haloarenes

EWG

$$Ar^{1}$$
-X

 $X = I, Br$ 
 $Ar^{1}$ -Ar<sup>2</sup>
 $Ar^{2}$ -Y

 $Y = B(OH)_{2}, SnBu_{3}$ 

EWG

 $Ar^{1}$ 
 $Ar^{1}$ 

# M.G. Buonomenna, L.C. Lopez, G. Barbieri, P. Favia, R. d'Agostino, E. Drioli

Journal of Molecular Catalysis A: Chemical 273 (2007) 32

Sodium tungstate immobilized on plasma-treated PVDF membranes: New efficient heterogeneous catalyst for oxidation of secondary amines to nitrones

## Mallikarjun V. Patil, Mukesh K. Yadav, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 273 (2007) 39

Prins condensation for synthesis of nopol from  $\beta$ -pinene and paraformaldehyde on novel Fe–Zn double metal cyanide solid acid catalyst

Contents vii

### F. Richard, T. Boita, M. Moreau, C. Bachmann, G. Pérot

Journal of Molecular Catalysis A: Chemical 273 (2007) 48

Transformation of thiophenic compounds over HY zeolite. Study of the acid-catalyzed isomerization and disproportionation mechanisms by quantum chemical calculations

Over a HY zeolite, the thiophenic compounds (2-methylthiophene, 3-methylthiophene, 2-methylbenzothiophene and 3-methylbenzothiophene) underwent both isomerization and disproportionation. The product selectivities obtained experimentally were rationalized on the basis of the calculated stabilities (B3LYP method) of the expected cationic intermediates. These calculations allowed to explain why 2-methylthiophene and 3-methylthiophene presented the same reactivity in isomerization. Moreover, the distribution of the dimethylthiophenes obtained by disproportionation of the methylthiophene isomers was in good agreement with the relative stabilities of the carbenium ions involved in these reactions.

DMT	Intermediate	Relative
product	carbenium ion	energy
2,3-DMT		4
2,4-DMT	S S	18
3,4-DMT	⟨ŢŢ,	62

#### S.Z. Mohamed Shamshuddin, N. Nagaraju

Journal of Molecular Catalysis A: Chemical 273 (2007) 55

Liquid phase transesterification of methyl salicylate and phenol over solid acids: Kinetic studies

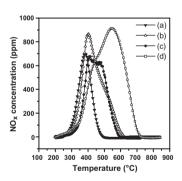
$$\begin{array}{c} C_{6}H_{4}(OH) \longrightarrow C \longrightarrow OMe & + & C_{6}H_{5}OH \\ \parallel & & \\ O & & \\ & & \\ ZrO_{2}, sulfated-ZrO_{2}, Mo(VI)/ZrO_{2} \\ \downarrow & & \\ C_{6}H_{4}(OH) \longrightarrow C \longrightarrow OC_{6}H_{5} & + & MeOH \\ \parallel & & \\ O & & \\ & &$$

#### Se Min Park, Ji Won Park, Heon-Phil Ha, Hyun-Sik Han, Gon Seo

Journal of Molecular Catalysis A: Chemical 273 (2007) 64

Storage of  $NO_2$  on potassium oxide co-loaded with barium oxide for  $NO_x$  storage and reduction (NSR) catalysts

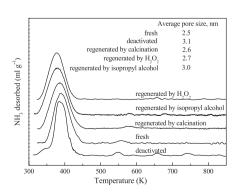
The strength of  $NO_2$  storage on barium oxide-based  $NO_x$  storage and reduction (NSR) catalysts is significantly enhanced by addition of potassium oxide. The TPD profiles of  $NO_2$  from (a)  $Al_2O_3$ , (b) BaO  $(0.50)/Al_2O_3$ , (c)  $K_2O$   $(0.40)/Al_2O_3$ , and (d)  $K_2O$  (0.70)–BaO  $(0.50)/Al_2O_3$  catalysts clearly show the role of barium oxide as a material for  $NO_2$  storage and that of potassium oxide in enhancing the interaction between  $NO_2$  and the NSR catalysts.



### Qingfa Wang, Li Wang, Junxia Chen, Yulong Wu, Zhentao Mi

Journal of Molecular Catalysis A: Chemical 273 (2007) 73

Deactivation and regeneration of titanium silicalite catalyst for epoxidation of propylene The addition by-products and dimeric compounds or oligomers of propylene oxide blocked the channels and covered the active sites, which mainly contributes to deactivation of the TS-1 catalyst. In addition, Ti leaching also occurred in the continuous epoxidation of propylene. The regeneration by calcination completely burnt off the coke deposition and the catalytic activity can be fully recovered except for that caused by Ti leaching.



viii Contents

#### Fengtao Chen, Hongzhu Ma, Bo Wang, Qiongfang Zhuo

Journal of Molecular Catalysis A: Chemical 273 (2007) 81

One-step production of methoxymethyl benzene in electrochemical reaction of toluene with methanol assisted by modified  $(NH_4)_3H_4[P(Mo_2O_7)_6]$  catalysts

A toluene free-radical cation formed in the oxidation of side-chain of toluene assisted by P, Mo metal-salt  $(M_x O_y - MoO_3 - P_2 O_5, M = Fe, Ni, Cu)$  catalysts then produce a free radical. All products were obtained by the reaction of the free radical with toluene or methanol. A possible free-radicals reaction mechanism confirmed by XPS and UV-vis spectra was proposed.

#### Anne-Sophie Rodrigues, Evgueni Kirillov, Bruno Vuillemin, Abbas Razavi, Jean-François Carpentier

Journal of Molecular Catalysis A: Chemical 273 (2007) 87

Binary ansa-lanthanidocenes/dialkylmagnesium systems versus single-component catalyst: Controlled synthesis of end-capped syndiotactic oligostyrenes

### A. Solladié-Cavallo, A. Baram, E. Choucair, H. Norouzi-Arasi, M. Schmitt, F. Garin

Journal of Molecular Catalysis A: Chemical 273 (2007) 92

Heterogeneous hydrogenation of substituted phenols over Al<sub>2</sub>O<sub>3</sub> supported ruthenium

Catalytic heterogeneous hydrogenation over  $Ru/Al_2O_3$  of mono- and di-substituted phenols works and provides mixtures of isomers, the all-cis isomers (corresponding to all-syn  $H_2$  additions) being always major.

1: 
$$R^{1}$$
=Me,  $R^{2}$ =H  
2:  $R^{1}$ =CO<sub>2</sub>Me,  $R^{2}$ =H  
3:  $R^{1}$ = $R^{2}$ =Me  
4:  $R^{1}$ =i-Pr,  $R^{2}$ =Me  
all-cis = major

# Majid M. Heravi, Khadijeh Bakhtiari, Zohreh Daroogheha, Fatemeh F. Bamoharram

Journal of Molecular Catalysis A: Chemical 273 (2007) 99

Facile heteropolyacid-promoted synthesis of 14-substituted-14-H-dibenzo[a,j] xanthene derivatives under solvent-free conditions

An efficient and facile synthesis of biologically active 14-substituted-14-H-dibenzo[a,j] xanthene derivatives were reported via three-component condensation reaction of  $\beta$ -naphthol and aldehydes in the presence of a catalytic amount of Preyssler type heteropoly acid, under solvent-free conditions. This method is very easy, rapid and high yielding reaction for the synthesis of dibenzo xanthene derivatives.

Contents ix

### Suman Sahoo, Pradeep Kumar, F. Lefebvre, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 273 (2007) 102

Immobilized chiral diamino Ru complex as catalyst for chemo- and enantioselective hydrogenation

Chiral cyclohexyldiamine based Ru triphenylphosphine complex immobilized over mesoporous silica SBA-15 was found to be highly active in the chemo- and enantioselective hydrogenation of prochiral,  $\alpha,\beta$ -unsaturated ketones and imines to corresponding products.

$$\begin{array}{c} X \\ R_1 \\ R_2 \end{array} \xrightarrow{\textbf{catalyst}} \begin{array}{c} XH \\ R_1 \\ X=N,O \end{array}$$

$$X=N,O$$

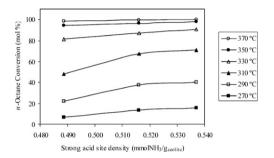
$$Y=N,O$$

#### Paula Sánchez, Fernando Dorado, Antonia Fúnez, Vicente Jiménez, María Jesús Ramos, José Luis Valverde

Journal of Molecular Catalysis A: Chemical 273 (2007) 109

Effect of the binder content on the catalytic performance of beta-based catalysts

The influence of the amount of a clay binder on the properties of beta zeolite based catalysts for the hydroisomerization of n-octane was studied. EFAL species were present on the agglomerated catalysts enhancing their acid strength through a synergetic effect that allowed them to be much more active for the hydroisomerization of n-octane.



### B.P. Bandgar, Abasaheb V. Patil, V.T. Kamble, J.V. Totre

Journal of Molecular Catalysis A: Chemical 273 (2007) 114

An efficient synthesis of thiiranes from oxiranes using fluoroboric acid adsorbed on silica gel (HBF $_4$ -SiO $_2$ ) as a catalyst under mild conditions in the absence of solvent

An efficient synthesis of thiiranes from oxiranes using a heterogeneous catalyst under solvent-free and mild conditions.

#### Christian Görl, Helmut G. Alt

Journal of Molecular Catalysis A: Chemical 273 (2007) 118

Iron complexes with  $\omega$ -alkenyl substituted bis(arylimino)pyridine ligands as catalyst precursors for the oligomerization and polymerization of ethylene

A series of 15 iron complexes with  $\omega$ -alkenyl functionalized bis(arylimino)pyridine ligands was synthesized and characterized. After activation with methylalumoxane (MAO), these catalysts oligomerize or polymerize ethylene to give highly linear products. Their potential for self-immobilization during the polymerization process was investigated.

$$R^3$$
 $R^4$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 
 $R^5$ 
 $R^4$ 
 $R^3$ 
 $R^2$ 
 $R^1$ 
 $R^2$ 
 $R^1$ 
 $R^2$ 
 $R^3$ 
 $R^2$ 

x Contents

### Mannar R. Maurya, Maneesh Kumar, Umesh Kumar

Journal of Molecular Catalysis A: Chemical 273 (2007) 133

Polymer-anchored vanadium(IV), molybdenum(VI) and copper(II) complexes of bidentate ligand as catalyst for the liquid phase oxidation of organic substrates

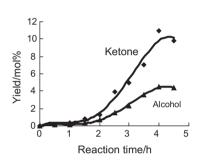
Polymer-anchored catalysts  $PS-[VO(hpbmz)_2]$ ,  $PS-[MoO_2(hpbmz)_2]$  and  $PS-[Cu(hpbmz)_2]$  (where Hhpbmz = 2-(2'-hydroxyphenyl)benzimidazole) have been prepared and characterised. These complexes catalyse the oxidation of styrene, ethylbenzene and methyl phenyl sulfide efficiently.

#### Guan Huang, Yong-An Guo, Hong Zhou, Shu-Kai Zhao, Shang-Yue Liu, Ai-Ping Wang, Jian-Feng Wei

Journal of Molecular Catalysis A: Chemical 273 (2007) 144

Oxidation of cyclohexane with a new catalyst  $(TPPFe^{III})_2O$  supported on chitosan

Chitosan-supported  $\mu$ -oxo dimeric iron tetraphenyl-porphyrin was used as catalyst for cyclohexane oxidation. It was found that the supported catalyst gave 13.0% yield and about 90% selectivity for ketone and alcohol, and a catalyst turnover number of 1.03  $\times$  10<sup>5</sup>. The supported catalyst can be efficiently reused six times and showed better performance than the unsupported catalyst for cyclohexane oxidation.



#### Prudence Tau, Tebello Nyokong

Journal of Molecular Catalysis A: Chemical 273 (2007) 149

Comparative photocatalytic efficiency of oxotitanium(IV) phthalocyanines for the oxidation of 1-hexene Oxotitanium(IV) phthalocyanine complexes photocatalyse the transformation of 1-hexene giving 1,2-epoxyhexane and 1-hexen-3-ol through Types II and I mechanisms.

$$H_3C$$
 $CH_2$ 
 $H_2C$ 
 $CH$ 
 $CH$ 

#### Mei-Jin Lin, Liang Yang, Jun-Dong Wang

Journal of Molecular Catalysis A: Chemical 273 (2007) 156

The spectra and stabilities of alkoxyl-substituted phthalocyaninatometals. I. The effect of axial coordination abilities of the center metals on their stabilities in benzoyl peroxide The stabilities of phthalocyaninatometals are reduced seriously by the substitution of bulky alkoxyl substituents. In the toluene, tetra- $\alpha$ -(2,2,4-trimethyl-3-pentoxy)phthalocyaninatometals can be decomposed by the benzoyl peroxide, and the order of decomposition rate sorted with the center metals is Fe > Co > Cu > Ni > Pd, which showed a consistency with the axial coordination abilities of the center metals.

Contents xi

### Xiaodong Wang, Minghui Liang, Hongquan Liu, Yuan Wang

Journal of Molecular Catalysis A: Chemical 273 (2007) 160

Selective hydrogenation of bromonitrobenzenes over Pt/ $\gamma$ -Fe $_2$ O $_3$ 

The  $Pt/\gamma$ -Fe<sub>2</sub>O<sub>3</sub> nanocomposite catalyst exhibited very excellent catalytic properties for selective hydrogenation of o-bromonitrobenzene, m-bromonitrobenzene and p-bromonitrobenzene to the corresponding bromonilines

$$Br$$
 $NO_2$ 
 $H_2$ 
 $Pt/\gamma - Fe_2O_3$ 
 $Br$ 
 $NH_2$ 
Selectivity: ~99.9%

#### Salam J.J. Titinchi, Fadhil S. Kamounah, Hanna S. Abbo

Journal of Molecular Catalysis A: Chemical 273 (2007) 169

Preparation of mono- and diacetyl 4,4'-dimethylbiphenyl and their corresponding carboxylic acids: Reactivity, selectivity and isomer distribution studies via Lewis acid catalyzed Friedel-Crafts acetylation/oxidation Shape selective acetylation of 4,4'-dimethylbiphenyl (DMBPh) with acetyl chloride using aluminum chloride anhydrous as catalyst is an effective route for the production of mono- and di-acetyl-isomers. Systematic study of the catalytic Friedel-Crafts acetylation of DMBPh was carried out in a range of solvents and under a variety of experimental conditions. The obtained ketones were converted to the corresponding carboxylic acids. 2-acteyl-4,4'-dimethylbiphenyl was prepared by indirect stepwise synthetic route. 3-D molecular modeling supports the positional assignment of the acetyl group with the results obtained from the electronic spectra.

# N. Venkatachalam, M. Palanichamy, V. Murugesan

Journal of Molecular Catalysis A: Chemical 273 (2007) 177

Sol-gel preparation and characterization of alkaline earth metal doped nano TiO<sub>2</sub>: Efficient photocatalytic degradation of 4-chlorophenol

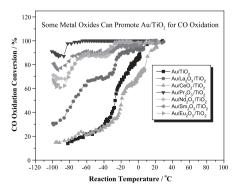
Nano  ${\rm TiO}_2$ ,  ${\rm Ba}^{2+}$  and  ${\rm Mg}^{2+}$  doped nano  ${\rm TiO}_2$  were prepared by sol-gel method using titanium(IV) isopropoxide, barium and magnesium nitrate as precursors. The materials were characterized by XRD, BET, FT-IR, TGA, UV-vis, SEM and TEM techniques. Photocatalytic degradation of 4-chlorophenol (4-CP) in aqueous solution was carried out using nano,  ${\rm Ba}^{2+}$  and  ${\rm Mg}^{2+}$  doped nano  ${\rm TiO}_2$ . Experimental results revealed that 1 mol%  ${\rm Ba}^{2+}$  and  ${\rm Mg}^{2+}$  doped nano  ${\rm TiO}_2$  required shorter irradiation time for complete mineralization of 4-CP than pure nano  ${\rm TiO}_2$  and commercial  ${\rm TiO}_2$  (Degussa P-25).

$$\begin{array}{c} OH \\ \hline \\ Ba^{2+}/Mg^{2+}-TiO_2 \\ \hline \\ CO_2 + H_2O + CI \\ \end{array}$$

#### Zhen Ma, Steven H. Overbury, Sheng Dai

Journal of Molecular Catalysis A: Chemical 273 (2007) 186

Au/M<sub>x</sub>O<sub>y</sub>/TiO<sub>2</sub> catalysts for CO oxidation: Promotional effect of main-group, transition, and rare-earth metal oxide additives Au/ ${\rm TiO_2}$  is the most studied gold catalyst for CO oxidation, but few attempts have been made to enhance its activity and thermal stability. In this report, we modified the  ${\rm TiO_2}$  support by an array of metal oxide additives followed by loading gold, and found drastic promotional effect caused by certain additives.



xii Contents

#### Tarek Mohamed Salama, Ibraheem Othman Ali, Mohamed Mokhtar Mohamed

Journal of Molecular Catalysis A: Chemical 273 (2007) 198

Synthesis and characterization of mordenites encapsulated titania nanoparticles: Photocatalytic degradation of *meta*-chlorophenol

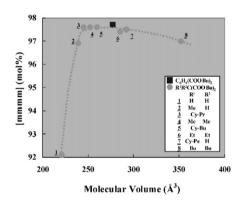
This scheme represents the steps of decomposing MCP photo-catalytically over  $TiM_{ss}$  catalyst describing that it undergoes to some aliphatic moieties before evolving  $CO_2$ .

#### Shohjiroh Tanase, Kiyokazu Katayama, Nobuhiro Yabunouchi, Takanori Sadashima, Norio Tomotsu, Nobuhide Ishihara

Journal of Molecular Catalysis A: Chemical 273 (2007) 211

Design of novel malonates as internal donors for MgCl<sub>2</sub>-supported TiCl<sub>4</sub> type polypropylene catalysts and their mechanistic aspects, Part 1

Propylene polymerization using MgCl<sub>2</sub>-supported TiCl<sub>4</sub> type catalysts with new various malonate compounds (R<sup>1</sup>R<sup>2</sup>C(COOBu)<sub>2</sub>) as internal donors was investigated. The catalytic activity and isotacticity of polypropylene (PP) depended on the molecular volume of the malonates. Furthermore, the mechanism of the active site formation was discussed with the catalyst compositions, the temperature rising elution fractionation curves of PP and so on.



# K. Shivakumar, M.K. Veeraiah, K.S. Rai, B.S. Sherigara, N.M. Made Gowda

Journal of Molecular Catalysis A: Chemical 273 (2007) 218

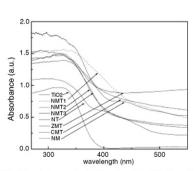
Kinetics of polymerization of acrylonitrile initiated by the vanadium(V)-bisulphite redox system in sulphuric and perchloric acid media The kinetics of polymerization of acrylonitrile, initiated by the free radicals formed in situ in the vanadium(V)-bisulphite redox system, was studied in aqueous sulphuric acid and perchloric acid media in the temperature range of  $28-40~^{\circ}$ C. The rate of polymerization was determined at various concentrations of the monomer and initiators. The effect of intermediate injection of catalyst was studied. The temperature dependence of the rate was studied and the activation parameters were computed. The resulting polymer (polyacrylonitrile (PAN)) was characterized by infrared (IR) and  $^{1}$ H NMR spectral analysis and by its molecular weight determined by the viscometric method. A possible mechanism consistent with the experimental data has been proposed.

### T.K. Ghorai, D. Dhak, S.K. Biswas, S. Dalai, P. Pramanik

Journal of Molecular Catalysis A: Chemical 273 (2007) 224

Photocatalytic oxidation of organic dyes by nano-sized metal molybdate incorporated titanium dioxide  $(M_x Mo_x Ti_{1-x} O_6)$  (M = Ni, Cu, Zn) photocatalysts

The calculated band-gap energy of  $Ni_xMo_xTi_{1-x}O_6$  (NMT1; x=0.05) from adsorption edge is found to be 2.66 eV and band-gap energy of other metal molybdenum doped  $TiO_2$   $M_xMo_xTi_{1-x}O_6$  (M = Ni, Cu, Zn; x=0.05) is calculated (shown in Table 1). As lower band gap and particle size (around 15 nm) of NMT1, so it can acts as a higher photocatalytic activity compare the other metal molybdenum doped  $TiO_2$  photocatalyst.



UV-visible diffuse reflectance spectra of M-Ti samples with the highest dopant-atom

Contents xiii

#### Laurent Djakovitch, Pascal Rouge

Journal of Molecular Catalysis A: Chemical 273 (2007) 230

New homogeneously and heterogeneously [Pd/Cu]catalysed C3-alkenylation of free NH-indoles

R = H, Me, Ph, CO<sub>2</sub>Me

58-82 % isolated yields

#### Kai Cheng, Bingwei Xin, Yuhong Zhang

Journal of Molecular Catalysis A: Chemical 273 (2007) 240

The Pd(OAc)2-catalyzed homocoupling of arylboronic acids in water and ionic liquid

The homocoupling reaction of the arylboronic acids is efficiently catalyzed by Pd(OAc)<sub>2</sub> in a mixture of water and ionic liquids in the presence of ethyl bromoacetate ester. Various symmetrical biaryls is synthesized in high yields in short reaction times and the Pd(OAc)<sub>2</sub>-[bmim][PF<sub>6</sub>] (1-butyl-3-methylimidazolium hexafluorophosphate) can be reused eight times only with a slight decrease in activity.

2 ArB(OH)<sub>2</sub> 
$$\frac{\text{Pd(OAc)}_2, [\text{bmim}][\text{PF}_6] - \text{H}_2\text{O}, 3 \text{ h}}{\text{K}_2\text{CO}_3, \text{ BrCH}_2\text{COOEt}, 60 °C} \qquad \text{Ar-Ar}$$
8 Recycles

#### P. Sangeetha, P. Seetharamulu, K. Shanthi, S. Narayanan, K.S. Rama Rao

Journal of Molecular Catalysis A: Chemical 273 (2007) 244

Studies on Mg-Al oxide hydrotalcite supported Pd catalysts for vapor phase hydrogenation of nitrobenzene

Hydrotalcite supported Pd catalyst with lower Pd content (0.5 wt.% Pd/HT) shows higher conversion of nitrobenzene with higher selectivity to aniline in the vapor phase hydrogenation of nitrobenzene to aniline at atmospheric pressure due to higher dispersion and smaller particle size as observed from CO chemisorption and XRD results.

$$NO_2$$
  $+ 3H_2$   $Pd/HT$   $+ 2H_2O$  Aniline

### Tatiana Luts, René Frank, Wladimir Suprun, Sebastian Fritzsche, Evamarie Hey-Hawkins, **Helmut Papp**

Journal of Molecular Catalysis A: Chemical 273 (2007) 250

Epoxidation of olefins catalyzed by novel Mn(III) and Mo(IV)-Salen complexes immobilized on mesoporous silica gel. Part II: Study of the catalytic epoxidation of olefins

Homogeneous Mn(III) and Mo(IV)-Salen complexes and those immobilized on a silica surface were studied in the catalytic epoxidation of cyclooctene and cyclohexene with tert-butylhydroperoxide (TBHP) and hydrogen peroxide (HP) as an oxidant.

xiv Contents

# T.C.O. Mac Leod, V.P. Barros, A.L. Faria, M.A. Schiavon, I.V.P. Yoshida, M.E.C. Queiroz, M.D. Assis

Journal of Molecular Catalysis A: Chemical 273 (2007) 259

Jacobsen catalyst as a P450 biomimetic model for the oxidation of an antiepileptic drug The carbamazepine oxidation by 3-chloroperoxybenzoic acid (m-CPBA), tert-butyl hydroperoxide (t-BuOOH) or  $H_2O_2$ , mediated by a salen complex was investigated in homogeneous medium or encapsulated in a matrix based on poly(dimethylsiloxane). The product carbamazepine 10,11-epoxide is dependent on the oxidant, pH, solvent and co-catalyst. The encapsulated complex was an efficient catalyst for carbamazepine oxidation using t-BuOOH and t-CPBA as oxidant.

$$O \longrightarrow NH_2$$

$$O \longrightarrow NH_2$$

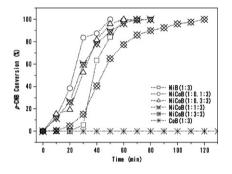
$$CBZ \qquad CBZ-EP$$

#### Jia-Huei Shen, Yu-Wen Chen

Journal of Molecular Catalysis A: Chemical 273 (2007) 265

Catalytic properties of bimetallic NiCoB nanoalloy catalysts for hydrogenation of *p*-chloronitrobenzene

Adding small amount of cobalt in the NiB catalysts increased the surface area and reaction activity, but decreased the selectivity for the desired product, *p*-CAN. However, overdosed cobalt had an opposite effect on the Ni catalyst, it reduced the reaction activity but increased the selectivity for *p*-CAN.

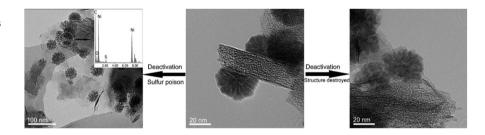


### Zhijie Wu, Minghui Zhang, Wei Li, Shicheng Mu, Keyi Tao

Journal of Molecular Catalysis A: Chemical 273 (2007) 277

Study on the deactivation of supported amorphous Ni-B catalyst in hydrogenation

The deactivation of supported Ni-B/MgO catalyst prepared by a modified electroless plating method was studied in the hydrogenation of sulfolene and acetophenone. The results showed that the deactivation of catalyst was due to the sulfur-poisoning and the destruction of the porous structure of Ni-B particles.



### Gui Chen, Yan Xing, Hui Zhang, Jing-Xing Gao

Journal of Molecular Catalysis A: Chemical 273 (2007) 284

Synthesis of novel chiral macrocyclic ONNO-type ligands and use in asymmetric transfer hydrogenation

$$R^{1} \stackrel{\text{[IrHCl}_{2}(COD)]_{2}}{}/L^{*}$$

$$KOH / iso-PrOH$$

$$R^{1} \stackrel{\text{[I}}{||}$$

$$R^{2} \stackrel{\text{Constant of } PrOH}{} R^{2} \stackrel{\text{C$$

Contents xv

#### Hiroyuki Komatsu, Bungo Ochiai, Tetsuo Hino, Takeshi Endo

Journal of Molecular Catalysis A: Chemical 273 (2007) 289

Thermally latent reaction of hemiacetal ester with epoxide controlled by Schiff-base-zinc chloride complexes with tunable catalytic activity

We describe a model reaction for a cross-linking system with high activity and latency catalyzed by a Schiffbase-zinc chloride complexes. The Schiff-base-zinc chloride complexes thermally-latently catalyze the addition of a hemiacetal ester and an epoxide through the thermal dissociation of the hemiacetal ester to a carboxylic acid and a vinyl ether, which takes place only at appropriate temperatures for cross-linking. This latent reaction shows both excellent latency under ambient conditions and high activity only at specific temperatures.

### Mohammed Al-Hashimi, Alice C. Sullivan, John R.H. Wilson

Journal of Molecular Catalysis A: Chemical 273 (2007) 298

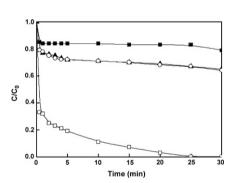
Palladium ethylthioglycolate modified silica—a new heterogeneous catalyst for Suzuki and Heck cross-coupling reactions A new silica supported sulfur containing ethylthioglycolate material that readily binds Pd from solutions of palladium acetate is reported. This affords an active and recyclable solid phase catalyst for Suzuki and Heck reactions with no evidence of Pd leaching.

### Teh-Long Lai, Wen-Feng Wang, Youn-Yuen Shu, Yi-Ting Liu, Chen-Bin Wang

Journal of Molecular Catalysis A: Chemical 273 (2007) 303

Evaluation of microwave-enhanced catalytic degradation of 4-chlorophenol over nickel oxides

A novel and environmentally friendly process for the degradation of 4-chlorophenol (4-CP) has been succeeded development with microwave-enhance catalytic degradation (MECD) method. Activity of 4-CP degraded is strongly dependent on the oxidation state of nickel and decreases slightly with the particle size of nickel oxide.



#### Mohammad Joshaghani, Elahe Faramarzi, Ezzat Rafiee, Marzieh Daryanavard, Jianliang Xiao, Colin Baillie

Journal of Molecular Catalysis A: Chemical 273 (2007) 310

Highly efficient Suzuki coupling using moderately bulky tolylphosphine ligands

Tolylphosphines,  $P(o\text{-tolyl})_n Ph_{3-n}$  promote efficiently the palladium catalyzed Suzuki cross-coupling reaction of arylboronic acids with aryl halides and bromoarylphosphine oxides with high conversions and turnovers.

$$X - \bigvee_{\substack{P \\ R^1}} + (HO)_2 B - \bigvee_{\substack{P \\ R^2}} - \frac{Pd \ catalyst}{Phosphine \ \textbf{I, II, III}}$$
Base,  $Bu_4NBr$ 
Solvent
$$R^1 - R^2$$

I: P(o-toly)Ph<sub>2</sub>, II: P(o-toly)<sub>2</sub>Ph, III: P(o-toly)<sub>3</sub>