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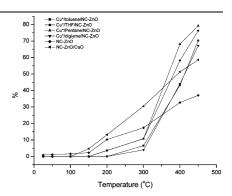
## Contents

### **Articles**

#### Aldo A. Ponce, Kenneth J. Klabunde

Journal of Molecular Catalysis A: Chemical 225 (2005) 1

Chemical and catalytic activity of copper nanoparticles prepared via metal vapor synthesis The chemical and catalytic activity of nanocrystal-line copper nanoparticles prepared using the solvated metal dispersion (SMAD) technique was studied. The Cu\*/toluene sample shows a yield of 90% toward the aryl homocoupling reaction of iodobenzene. A conversion of 80% was obtained for the Cu\*/pentane/NC-ZnO sample during the hydrogenation of CO<sub>2</sub> to form CH<sub>3</sub>OH.



#### Agnieszka Bukowska, Wiktor Bukowski, Jarosław Noworól

Journal of Molecular Catalysis A: Chemical 225 (2005) 7

Catalytic activity of salenCo(III)OAc complex in the reaction of addition of carboxylic acids to terminal epoxides The catalytic activity and regioselectivity were studied of the salenCo(III)OAc complex in the reaction of addition of aliphatic carboxylic acids (2) to a series of terminal epoxides (3). The reduction in the activity in the order: acetic > acrylic > methacrylic acid was found. The regioselectivity of the addition was independent on carboxylic acid nature and depended on the nature of the epoxide.

#### Giorgio Chelucci, Daniele Muroni, Ilaria Manca

Journal of Molecular Catalysis A: Chemical 225 (2005) 11

Enantioselective reduction of acetophenone with PMHS and tin(II) complexes of chiral pyridine ligands

A number of tin(II) complexes, prepared in situ from tin(II) triflate and pyridine derivatives (2,2':6',2"-terpyridine, 1,10-phenanthroline, 2,2'-bipyridine, dipyridylmethane, 2-(thiophen-2-yl)pyridine and 2-(2-diphenylphosphinophenyl)-5,6,7,8-tetrahydroquinoline), have been used as chiral catalysts for the reduction of acetophenone in the presence of polymethylhydrosiloxane (PMHS). Yields up to 82% and enantioselectivities up to 19% have been obtained.

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Mannepalli Lakshmi Kantam, Kalluri Venkata Sri Ranganath, Mutyala Sateesh, Kota Balaji Shiva Kumar, Boyapati Manoranjan Choudary

Journal of Molecular Catalysis A: Chemical 225 (2005) 15

Friedel-Crafts acylation of aromatics and heteroaromatics by beta zeolite

The Friedel–Crafts acylation of aromatic compounds such as anisole, 2-methoxynaphthalene, veratrole, isobutylbenzene and aromatic heterocycle compounds such as pyrrole, furan, thiophene, benzothiophene with different acid anhydrides is carried out in the batch mode with different forms of beta zeolite. The micronized beta zeolite shows manifold activity over normal zeolite in acylation reactions of aromatics.

#### Marco Burgener, Tamas Mallat, Alfons Baiker

Journal of Molecular Catalysis A: Chemical 225 (2005) 21

Palladium-catalysed dehydrogenation of 1-phenylethanol in dense carbon dioxide High rate and selectivity were achieved in a continuous flow reactor in dense CO<sub>2</sub> at around 150 °C, without any catalyst deactivation.

## Jianzhou Gui, Hongyan Ban, Xiaohui Cong, Xiaotong Zhang, Zhide Hu, Zhaolin Sun

Journal of Molecular Catalysis A: Chemical 225 (2005) 27

Selective alkylation of phenol with *tert*-butyl alcohol catalyzed by Brönsted acidic imidazolium salts SO<sub>3</sub>H-functionalized ionic liquids could be an efficient catalyst for the alkylation of phenol with *tert*-butyl alcohol (TBA) and were found to catalyze this reaction with good conversion and selectivity.

OH 
$$+$$
 HO  $+$  HSO<sub>4</sub>  $+$  HO  $+$  OH OH OH  $+$  OH  $+$ 

## Jincheng Mao, Boshun Wan, Zhanjin Zhang, Rongliang Wang, Fan Wu, Shiwei Lu

Journal of Molecular Catalysis A: Chemical 225 (2005) 33

Reversal of enantioselectivity by adding Ti(O<sup>f</sup>Pr)<sub>4</sub>: novel sulfamide-amine alcohol ligands for the catalytic asymmetric addition of diethylzinc to aldehydes

Novel sulfamide-amine alcohols (6) were applied to the catalytic asymmetric addition of diethylzinc to aldehydes, providing (S)-products in high yields and good enantioselectivities. These sulfamide-amie alcohols together with  $\mathrm{Ti}(\mathrm{O}^i\mathrm{Pr})_4$  were shown to obtain the (R)-products in significant enantiomeric excesses and high yields.

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### Lúcia K. Noda, Rusiene M. de Almeida, Luiz Fernando D. Probst, Norberto S. Gonçalves

Journal of Molecular Catalysis A: Chemical 225 (2005)39

Characterization of sulfated TiO2 prepared by the sol-gel method and its catalytic activity in the nhexane isomerization reaction

Sulfated TiO2 samples prepared by sol-gel method with some variations in the preparation conditions were characterized by thermal analysis, infrared and Raman spectroscopy, Brönsted/Lewis surface acid sites ratio determination by infrared spectra of pyridine adsorption and surface area and pore diameter analysis. The most active samples for n-hexane isomerization were those with higher Brönsted/Lewis acid ratio and higher proportion of pore diameter above 40.

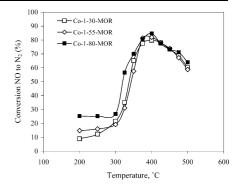
n-hexane conversion (%) at 100°C on sol-gel prepared sulfated TiO,

#### A. De Lucas, J.L. Valverde, F. Dorado, A. Romero, I. Asencio

Journal of Molecular Catalysis A: Chemical 225 (2005)47

Influence of the ion exchanged metal (Cu, Co, Ni and Mn) on the selective catalytic reduction of NO<sub>X</sub> over mordenite and ZSM-5

SCR of NO by propene was investigated on metal ion-exchanged zeolites. Co-Mordenite was found to be very active. NO TOF for all the catalysts were well correlated by a unique curve.

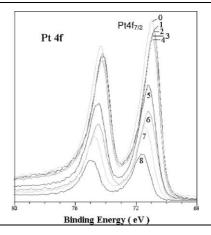


## Min Zhang, Zhensheng Jin, Jingwei Zhang, Zhijun Zhang, Hongxin Dang

Journal of Molecular Catalysis A: Chemical 225 (2005) 59

Effect of calcination and reduction treatment on the photocatalytic activity of CO oxidation on Pt/  $TiO_2$ 

The optimum calcination temperature of CO photocatalytic oxidation on Pt/TiO2 was 673 K. XPS results show after calcinating at 673 K, Pt doped into TiO2 lattice which can greatly enhance the CO photocatalytic activity.



## Kuan Xin Wang, Han Fei Xu, Wen Sheng Li, Xiao Ping Zhou

Journal of Molecular Catalysis A: Chemical 225 (2005) 65

Acetic acid synthesis from methane by non-synthesis gas process

Acetic acid was synthesized from a two-step process. In the first step, methane reacted with the water solution of HBr and oxygen to form CO and CH3Br over RuCl3/SiO2 catalyst, and in the second step, CH<sub>3</sub>Br reacted with CO and water to synthesize acetic acid over RhCl<sub>3</sub> catalyst.

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#### Benjaram M. Reddy, Pavani M. Sreekanth, Vangala R. Reddy

Journal of Molecular Catalysis A: Chemical 225 (2005) 71

Modified zirconia solid acid catalysts for organic synthesis and transformations

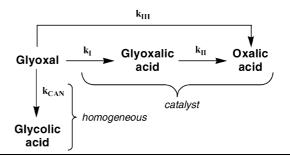
The sulfate, molybdate and tungstate promoted  $ZrO_2$  catalysts were investigated by X-ray diffraction, NH<sub>3</sub>-TPD, and Raman spectroscopy and were evaluated for various organic synthesis and transformation reactions. All catalysts exhibit good catalytic activity for synthesis of diphenylureas, coumarines and 1,5-benzodiazepines, acylation of alcohols, phenols and amines, and protection of carbonyl compounds.

# F. Alardin, H. Wullens, S. Hermans, M. Devillers

Journal of Molecular Catalysis A: Chemical 225 (2005) 79

Mechanistic and kinetic studies on glyoxal oxidation with Bi- and Pb-promoted Pd/C catalysts

The oxidation of glyoxal with bimetallic Pd–M/C catalysts (M = Bi, Pb) has been studied as a function of time. It was found that both Bi and Pb act as promoters, with an optimum corresponding to Pd/M = 1. The rate constants for each step of the complex reaction scheme were determined, giving useful mechanistic insight into the overall process.



Stanisław Krompiec, Mariola Pigulla, Nikodem Kuźnik, Michał Krompiec, Bogdan Marciniec, Dariusz Chadyniak, Janusz Kasperczyk

Journal of Molecular Catalysis A: Chemical 225 (2005) 91

Highly selective isomerization of *N*-allylamides catalyzed by ruthenium and rhodium complexes

Isomerization of N-allylamides (R<sup>1</sup>CON(R<sup>2</sup>)allyl) catalyzed by ruthenium and rhodium complexes has been studied. The first catalytic system containing a precursor ({[RuCl<sub>2</sub>(1,5-COD)]<sub>x</sub>}), tris(2,4-di-t-butylphenyl)phosphite and CaH<sub>2</sub> for highly (Z)-selective isomerization of allylamides is presented. It is suggested that the observed (Z)-selectivity of the isomerization of some allylamides is the result of the steric effect in the transition state.

$$\begin{array}{c|c}
O \\
R^{1} \\
N \\
B^{2}
\end{array}$$

$$\begin{array}{c|c}
\hline
(Ru] + L + CaH_{2} \\
\hline
a - d
\end{array}$$

$$\begin{array}{c}
O \\
N \\
R^{2}
\end{array}$$

a)  $R^1 = CH_3$ ,  $R^2 = H$ ,  $80^{\circ}C/2h$ , THF; b)  $R^1 = Ph$ ,  $R^2 = H$ ,  $90^{\circ}C/4h$ , THF; c)  $R^1 = NH_2$ ,  $R^2 = H$ ,  $100^{\circ}C/1h$ , 1,4-dioxane; d)  $R^1 = CH_3$ ,  $R^2 = Bu$ ,  $110^{\circ}C/2h$ , 1,4-dioxane;  $[Ru] = \{RuCl_2(1,5\text{-COD})]_x\}$ ; L = tris(2,4-di-t-butylphenyl) phosphite; amide : [Ru] : L :  $CaH_2 = 100$  : 1 : 1 : 10

# Takayuki Nagataki, Yoshimitsu Tachi, Shinobu Itoh

Journal of Molecular Catalysis A: Chemical 225 (2005) 103

Synthesis, characterization, and catalytic oxygenation activity of dinuclear iron(III) complex supported by binaphthol-containing chiral ligand

A  $(\mu$ -oxo)( $\mu$ -carboxylato) doubly bridged diiron(III) complex supported by a new dinucleating ligand containing a chiral binaphthol spacer has been synthesized and characterized. Catalytic oxidation of alkanes with m-CPBA proceeded very efficiently to give the corresponding alcohols as the major products together with ketones as minor products. Mechanistic studies have suggested that the reaction involves a highly reactive metal-based oxidant.

Contents ix

#### Brian P. Buffin, James P. Clarkson, Nadine L. Belitz, Abhijit Kundu

Journal of Molecular Catalysis A: Chemical 225 (2005) 111

Pd(II)-biquinoline catalyzed aerobic oxidation of alcohols in water

An aqueous palladium catalyst that is stabilized by a water-soluble biquinoline-based ligand was employed for the aerobic oxidation of secondary and primary alcohols. Secondary alcohols afforded the corresponding ketones while aliphatic primary alcohols were fully oxidized to carboxylic acid products. Water is used as the only reaction solvent and air is used as the oxidant, thus these conversions could serve as environmentally benign "green" alternatives to traditional oxidation methods.

#### S. Al-Khattaf, A. Iliyas, A. Al-Amer, T. Inui

Journal of Molecular Catalysis A: Chemical 225 (2005) 117

The effect of Y-zeolite acidity on *m*-xylene transformation reactions

It was found that the high acidity of H-Y-zeolite increases paring reaction, in addition to the well-known isomerization and disproportionation pathways. A significant drop in trimethyl-benzenes (TMBs) yields and a rise in benzene, gases and coke yields were observed with both reaction temperature and catalyst acidity. The *p*-xylene/*o*-xylene (P/O) ratio was found to be independent of zeolite acidity.

$$\bigcap_{G_1} \cdot C_{G_1} \xrightarrow{G_1} \bigcap_{G_2} \bigcap_{G_3} \bigcap_{G_3} \bigcap_{G_4} \bigcap_{$$

Reaction mechanism during m-xylene transformation.

## Kouji Takata, Sho-ta Yamaguchi, Satoru Nishiyama, Shigeru Tsuruya

Journal of Molecular Catalysis A: Chemical 225 (2005) 125

Cu precipitate formed during the benzene oxidation catalyzed by supported Cu in the presence of ascorbic acid and  $\rm O_2$ 

The Cu precipitate formed during the liquid-phase oxidation of benzene to phenol with supported Cu catalyst in the presence of  $O_2$  and ascorbic acid was confirmed to be a Cu oxalate analogue  $(Cu^{1+}[OC(=O)C(=O)OH]^{1-})$ , of which  $Cu^{1+}$  species were thought to be the cause of the deactivation of the benzene oxidation.

### Wei Juan Zhao, Xuan Zhen Jiang, Guang Lan Zhuo

Journal of Molecular Catalysis A: Chemical 225 (2005) 131

Selective carbonylation of benzene to benzaldehyde using  $O_2$  as the oxidant in the presence of cobalt complex

An efficient strategy on facial, environmentally friendly, economic, selective carbonylation of benzene to give benzaldehyde using  $O_2$  as the oxidant was firstly developed.

+ CO 
$$\frac{\text{Co(OAc)}_2}{\text{O}_2, \text{CCl}_3\text{COOH}, pyridine}$$