



Journal of Molecular Catalysis A: Chemical 280 (2008) v-xii

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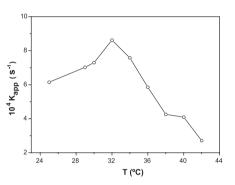
# Contents

# Articles

# Yao Wang, Guanwei Wei, Fei Wen, Xu Zhang, Wangqing Zhang, Linqi Shi

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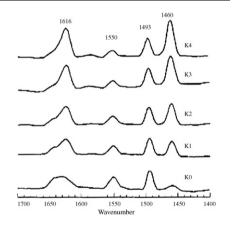
Synthesis of gold nanoparticles stabilized with poly-(*N*-isopropylacrylamide)-*co*-poly(4-vinyl pyridine) colloid and their application in responsive catalysis The catalyst of gold nanoparticles stabilized with thermoresponsive poly(N-isopropylacrylamide)co-poly(4-vinylpyridine) colloid was synthesized. The reduction of 4-nitrophenol with NaBH<sub>4</sub> via the catalyst was modulated due to the thermoresponsive phase-transition of the colloid-stabilizing gold nanoparticles. That was, the catalytic reduction firstly accelerated with the increase in temperature below the cloud-point temperature and then decelerated with the increase in temperature above the cloud-point temperature of the thermoresponsive colloid-stabilizing Au nanoparticles.



#### Jun Feng Liu, Yuan Liu, Liang Fu Peng

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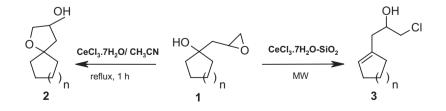
Aromatization of methane by using propane as coreactant over cobalt and zinc-impregnated HZSM-5 catalysts The TPD–NH<sub>3</sub> spectrum shows that the progressive shift to higher peak temperatures for low-temperature peak as cobalt concentration in the catalysts increased. The IR spectra in the pyridine region (1410–1575 cm<sup>-1</sup>) shows that as Co and Zn concentration in the catalyst increased the intensity of the band at 1550 cm<sup>-1</sup> (Bronsted acid sites) decreased a little and an increase of the intensity of the band at 1460 and 1616 cm<sup>-1</sup> (Lewis acid sites).



#### Gowravaram Sabitha, V. Rama Subba Rao, K. Sudhakar, M. Raj Kumar, E. Venkata Reddy, J.S. Yadav

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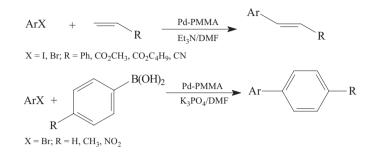
Study of conventional *versus* microwave-assisted reactions of 3,4-epoxyalcohols by  $CeCl_3 \cdot 7H_2O$ : Synthesis of tetrahydrofurans and 1-chloro-3-substituted-2-propanols



#### Dan Song, Wen-Bin Yi

Journal of Molecular Catalysis A: Chemical 280 (2008) 20

Polymethyl methacrylate micro-spheres supported palladium: A new catalyst for Heck and Suzuki reactions Commercially available polymethyl methacrylate (PMMA) micro-spheres supported palladium catalyses the highly efficient Heck and Suzuki cross-coupling reactions. The reactions can be performed under ligand-free conditions in an air atmosphere. The palladium catalyst is easily separated and can be reusable with negligible leaching of palladium.

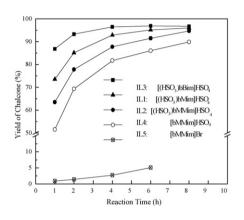


#### Jianghan Shen, Hua Wang, Hongchao Liu, Ying Sun, Zhongmin Liu

Journal of Molecular Catalysis A: Chemical 280 (2008) 24

Brønsted acidic ionic liquids as dual catalyst and solvent for environmentally friendly synthesis of chalcone

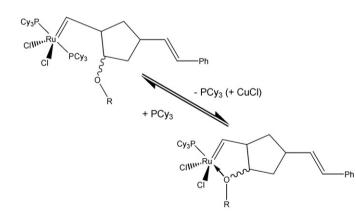
Brønsted acidic ionic liquids (ILs) as dual catalyst and solvent offer potential substitute for conventional homogenous/heterogeneous catalysts and solvent for Claisen–Schmidt(CS) condensation between acetophenone and benzaldehyde to produce chalcones. The ILs showed good catalytic activities and recycle capabilities. Both the structure of cation and anion of ILs could affect the activity of ILs. The optimized reaction conditions were investigated.



# Izabela Czelusniak, Joseph D. Heywood, Alan M. Kenwright, Ezat Khosravi

Journal of Molecular Catalysis A: Chemical 280 (2008) 29

Investigation of factors affecting ruthenium complexation in ROMP reactions of oxygen-containing norbornene derivatives using Grubbs first generation initiator

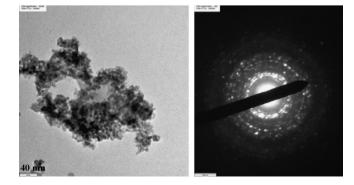


#### Watcharapong Khaodee, Bunjerd Jongsomjit, Piyasan Praserthdam, Shigeo Goto, Suttichai Assabumrungrat

Journal of Molecular Catalysis A: Chemical 280 (2008) 35

Impact of temperature ramping rate during calcination on characteristics of nano- $ZrO_2$  and its catalytic activity for isosynthesis

The effect of the temperature ramping rate during calcination on characteristics of nanoscale zirconia and its catalytic performance for isosynthesis was examined.

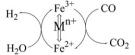


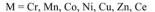
#### Ataullah Khan, Panagiotis G. Smirniotis

Journal of Molecular Catalysis A: Chemical 280 (2008) 43

Relationship between temperature-programmed reduction profile and activity of modified ferritebased catalysts for WGS reaction A series of modified ferrites prepared by doping iron oxide with various transition/non-transition/ inner-transition metal ions [M = Cr, Mn, Co, Ni, Cu, Zn and Ce] *in situ* during synthesis, were evaluated for WGS reaction. From TPR it was observed that, incorporation of metal cations into the hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) crystal structure alters the reducibility of the hematite particles, which in turn depends on the nature of the incorporated metal cation. A plausible explanation for the WGS activity over various modified ferrites has been attempted with the help of TPR analyses.

Dopant Promoted Fe<sup>2+</sup> --- Fe<sup>3+</sup> Redox Couple and Eventual WGS Activity Relationship

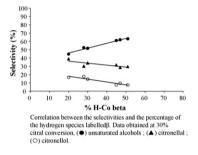




#### K. Kouachi, G. Lafaye, C. Especel, O. Cherifi, P. Marécot

Journal of Molecular Catalysis A: Chemical 280 (2008) 52

Effects of support and metal loading on the characteristics of Co based catalysts for selective hydrogenation of citral Silica-, alumina- and titania-supported Co catalysts were tested for selective citral hydrogenation. Three factors were found to be crucial to achieving high selectivity to unsatutared alcohols in the course of citral hydrogenation. These factors include a particular H-Co species (labelled  $\beta$ ), the Co<sup>0</sup> hexagonal phase and a large size of particles.

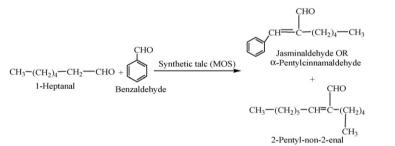


# Sumeet K. Sharma, Hasmukh A. Patel, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 280 (2008) 61

Synthesis of jasminaldehyde using magnesium organo silicate as a solid base catalyst

The amine/diamine functionalized synthetic talc (magnesium organo silicates; MOS) was synthesized by sol-gel method under non-hydrothermal conditions and used as a solid base catalyst for synthesis of jasminaldehyde. The highest conversion of 1-heptanal (99%) with 82% selectivity of jasminaldehyde was achieved using MOS3 as a catalyst.

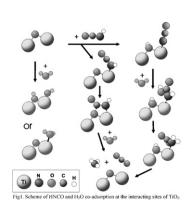


#### Izabela Czekaj, Oliver Kröcher, Gaia Piazzesi

Journal of Molecular Catalysis A: Chemical 280 (2008) 68

DFT calculations, DRIFT spectroscopy and kinetic studies on the hydrolysis of isocyanic acid on the  $TiO_2$ -anatase (1 0 1) surface

The co-adsorption of isocyanic acid (HNCO) and water ( $H_2O$ ) and their reaction to ammonia and carbon dioxide on the anatase phase of TiO<sub>2</sub> were studied with *ab initio* density functional theory (DFT) calculations using a cluster model as well as with *in situ* DRIFTS investigations and kinetic experiments.

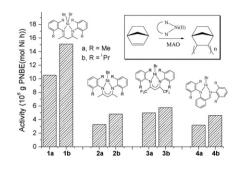


#### Haiyang Gao, Lixia Pei, Yongfei Li, Junkai Zhang, Qing Wu

Journal of Molecular Catalysis A: Chemical 280 (2008) 81

Vinyl polymerization of norbornene with nickel catalysts bearing [N,N] six-membered chelate ring: Important influence of ligand structure on activity

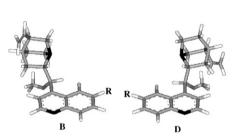
Vinyl polymerizations of norbornene with nickel complexes bearing [N,N] six-membered chelate ring activated with methylaluminoxane are investigated. The bulky steric hindrance of nickel complexes resulted in higher catalytic activity; ligands led to different electrophilicity of the nickel metal center, and a relatively positive nickel metal center would exhibit high catalytic activities for norbornene polymerization.



#### Katalin Balázsik, Imre Bucsi, Szabolcs Cserényi, György Szöllősi, Mihály Bartók

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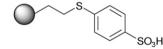
Methylethers of cinchona alkaloids in Pt-catalyzed hydrogenation of ethyl pyruvate and ketopantolactone: Effect of stereochemical factors on the enantioselectivity According to the new experimental data, it may be supposed that a two-point binding between reactant and chiral modifier is a prerequisite of the formation of the substrate–modifier 1:1 intermediate complex on platinum surface which is responsible for high ee's.



#### Amanmammet Bugrayev, Nazli Al-Haq, Rukeme A. Okopie, Asma Qazi, Michael Suggate, Alice C. Sullivan, John R.H. Wilson

Journal of Molecular Catalysis A: Chemical 280 (2008) 96

Covalently linked ethylmercaptophenyl sulfonic acid and ethylmercaptobenzyl sulfonic acid silica materials—Synthesis and catalytic activity In this paper we report on new silica immobilized ethylmercaptophenyl and ethylmercaptobenzyl sulfonic acid catalysts where the position of the sulfide group has a marked effect on the stability of the catalyst. The mercaptophenylsulfonic acid catalysts are thermally robust and highly efficient for a range of transformations including, esterification, etherification and carbonyl group protection. An apparent pore size effect on rate of conversion was observed. The mercaptobenzylsulfonic acid materials were comparatively unstable.



Excellent activity displayed in, esterification, transesterification, condensation and carbonyl group protection chemistries

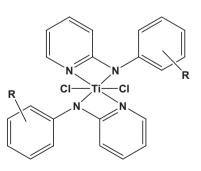


# Markku Talja, Mika Polamo, Markku Leskelä

Journal of Molecular Catalysis A: Chemical 280 (2008) 102

Bis(alkylphenylaminopyridinato) titanium dichlorides as ethylene polymerization catalysts

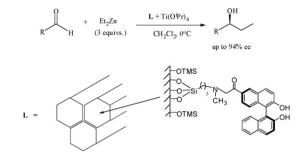
Four titanium alkylphenylaminopyridinato complexes were prepared and characterized by NMR. The complexes showed catalytic activity in the polymerization of ethylene when activated with MAO. The alkyl substituted complexes were less active, produced higher molar mass and broader molar mass distribution than phenylaminopyridinato complex. The fluxional behavior of the titanium aminopyridinato catalysts was the probable reason for the broad molar mass distribution.



# Kavita Pathak, Irshad Ahmad, Sayed H.R. Abdi, Rukhsana I. Kureshy, Noor-ul H. Khan, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 280 (2008) 106

The synthesis of silica-supported chiral BINOL: Application in Ti-catalyzed asymmetric addition of diethylzinc to aldehydes Silica-supported chiral BINOL was synthesized on two different pore sized mesoporous silica (SBA-15 (7.5 nm) and MCF (14 nm)), and shown to be highly active with an excellent enantioselectivity (up to 94% ee) in Ti-catalyzed asymmetric addition of diethylzinc to aldehydes. The MCF supported catalyst was reused in multiple catalytic runs without loss of enantioselectivity.

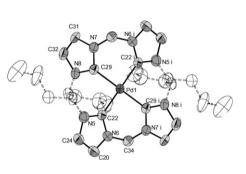


#### Chen-Shiang Lee, Sachindranath Pal, Wei-Shiuan Yang, Wen-Shu Hwang, Ivan J.B. Lin

Journal of Molecular Catalysis A: Chemical 280 (2008) 115

Bis-chelate tetracarbene palladium(II) complex as an efficient and recyclable catalyst precursor for Heck reaction

A homoleptic Pd(II) complex with two chelating di-*N*-heterocyclic carbene (NHC) ligands has been synthesized and its square planar molecular geometry has been determined by X-ray diffraction analysis. The complex proved to be an efficient catalyst having exceedingly high turnover number and good reusability in Heck reaction.

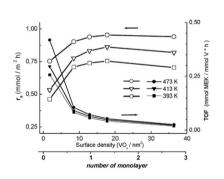


# Thomas Machold, Wladimir Y. Suprun, Helmut Papp

Journal of Molecular Catalysis A: Chemical 280 (2008) 122

Characterization of  $\mathrm{VO}_x\text{-}\mathrm{TiO}_2$  catalysts and their activity in the partial oxidation of methyl ethyl ketone

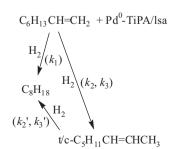
The present work focuses on the partial oxidation of methyl ethyl ketone to acetic acid over  $\text{TiO}_2$ supported vanadia catalysts with V loadings from 1 to 13.5 wt.%. The investigations showed that with increasing V loading the rate of MEK conversion increased whereas the turn-over frequency decreased (Fig. 7). The highest selectivities to acetic acid were achieved at V loadings of 4–6 wt.%.



#### Vasco F.D. Álvaro, Robert A.W. Johnstone

Journal of Molecular Catalysis A: Chemical 280 (2008) 131

High surface area Pd, Pt and Ni ion-exchanged Zr, Ti and Sn(IV) phosphates and their application to selective heterogeneous catalytic hydrogenation of alkenes Catalysts of  $Pd^0$ ,  $Pt^0$  and  $Ni^0$  were synthesised from large surface area Ti, Sn and Zr metal(IV) phosphates. The catalysts were examined for activity and selectivity towards heterogeneous liquid and gas phase hydrogenation of a variety of alkenes at room and elevated temperatures, in comparison with commercial Pd/C catalysts. Rate constants were determined.

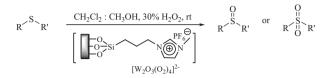


have been observed for the branched aldehyde.

#### Xian-Ying Shi, Jun-Fa Wei

Journal of Molecular Catalysis A: Chemical 280 (2008) 142

Selective oxidation of sulfide catalyzed by peroxotungstate immobilized on ionic liquid-modified silica with aqueous hydrogen peroxide Several sulfides were selectively oxidized to sulfoxides and sulfones with  $H_2O_2$  catalyzed by peroxotungstate immobilized on ionic liquid-modified silica. These recoverable catalysts both exhibit high catalytic activities in the oxidation reaction and provide excellent chemselectivities towards sulfur groups with unsaturated double bonds. The yields of methyl phenyl sulfoxide were still satisfied when the catalyst was reused for a sixth time.



#### Giulia Erre, Stephan Enthaler, Kathrin Junge, Serafino Gladiali, Matthias Beller

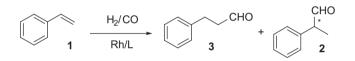
Journal of Molecular Catalysis A: Chemical 280 (2008) 148

Novel rhodium catalyst for asymmetric hydroformylation of styrene: Study of electronic and steric effects of phosphorus seven-membered ring ligands



The asymmetric hydroformylation of styrene catalysed by rhodium complexes modified by monodentate

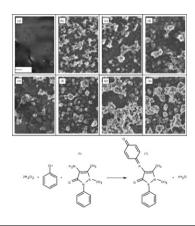
phosphepine ligands has been investigated. Regioselectivity up to 96% and enantioselectivity up to 48%



### R.R. Carballo, V. Campodall' Orto, I.N. Rezzano

Journal of Molecular Catalysis A: Chemical 280 (2008) 156

Supported bimetallic polymers of porphyrins as new heterogeneous catalyst

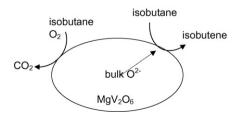


### Yusaku Takita, Susumu Hikazudani, Kazuya Soda, Katsutoshi Nagaoka

Journal of Molecular Catalysis A: Chemical 280 (2008) 164

Anaerobic oxidation of isobutane: Catalytic properties of  $MgV_2O_6$  and  $Mg_2V_2O_7$  prepared by the molten method

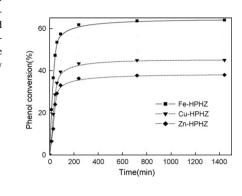
 $CuV_2O_6$ ,  $Co_2V_2O_7$  and  $Mg_{1.8}Cu_{0.2}V_2O_7$  prepared by molten method are suitable oxides for a thin layer reactor for anaerobic oxidation of isobutane. Two types of oxidations occurred simultaneously: isobutene formation by the lattice oxygen ions diffused from the bulk, and CO and CO<sub>2</sub> formation by the oxygen species derived from molecular oxygen in the gas phase.



#### K.C. Gupta, A.K. Sutar

Journal of Molecular Catalysis A: Chemical 280 (2008) 173

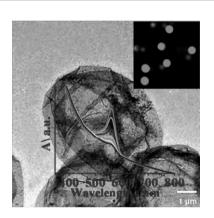
Polymer supported catalysts for oxidation of phenol and cyclohexene using hydrogen peroxide as oxidant The polymer supported HPHZ Schiff complexes of iron(III), copper(II) and zinc(II) ions were synthesized and used as catalyst in oxidation of phenol and epoxidation of cyclohexene in comparison to unsupported Schiff base complexes of metal ions. The supported catalysts showed high catalytic activity and product selectivity than unsupported catalysts.



# Xia Tao, Jingmei Su, Lingxuan Wang, Jian-Feng Chen

Journal of Molecular Catalysis A: Chemical 280 (2008) 186

A new heterogeneous catalytic system for wastewater treatment: Fe-immobilized polyelectrolyte microshells for accumulation and visible lightassisted photooxidative degradation of dye pollutants Fe-immobilized polyelectrolyte microshells constructed through the LbL self-assembly technique were verified to be effective in the accumulation of dye pollutants in water system and subsequent visible light-assisted degradation by  $H_2O_2$ . The stable performance and the accumulating capacity to organic species renders the Fe-immobilized microshells potentially applicable in the economical treatment of dye pollutants in natural aqueous ecosystems.



#### Rolando Roque-Malherbe, F. Diaz-Castro

Journal of Molecular Catalysis A: Chemical 280 (2008) 194

Calculation of the energy of adsorption of n-paraffins in nanoporous crystalline and ordered acid catalysts, and its relationship with the activation energy of the monomolecular catalytic cracking reaction

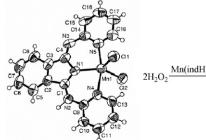


#### József Kaizer, Tamás Csay, Péter Kővári, Gábor Speier, László Párkányi

Journal of Molecular Catalysis A: Chemical 280 (2008) 203

Catalase mimics of a manganese(II) complex: The effect of axial ligands and pH

Catalase mimics of a manganese(II) complex: the effect of axial ligands and pH. The mononuclear  $[Mn(indH)Cl_2](CH_3OH)$  (indH: 1,3-bis(2'-pyridylimino)isoindoline) complex has been prepared and found to be suitable catalyst for the catalytic disproportionation of  $H_2O_2$  into  $H_2O$  and  $O_2$ .



 $2H_2O_2 \xrightarrow{Mn(indH)Cl_2} 2H_2O + O_2$ 

# Bing Yuan, Zongshi Li, Yongjun Liu, Shusheng Zhang

Journal of Molecular Catalysis A: Chemical 280 (2008) 210

Liquid phase acylation of 2-methylnaphthalene catalyzed by H-beta zeolite

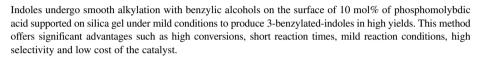
Liquid phase Friedel–Crafts acylation of 2-methylnaphthalene (2-MN) has been investigated over zeolite catalyst. The influence of zeolite structures, substituents on naphthalene, acylating agents and solvents on the acylation has been discussed. 2-Methyl-6-butyrylnaphthalene (2,6-BMN), a promising precursor of 2,6-naphthalenedicarboxylic acid (2,6-NDCA), has been synthesized by the acylation of 2-MN using butyric anhydride (BA) as an acylating agent and H-beta zeolite as a catalyst. The influence of the preparative methods and dosage of H-beta zeolite, the molar ratio of reactants, the reaction temperature and reaction time on the catalytic butyrylation was also studied. The H-beta zeolite exchanged for four times and calcined at 550 °C possessed relatively better catalytic performance. Under the optimized condition, the conversion of BA reached 78.3% and the selectivity for 2,6-BMN was 53.1%.

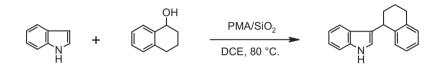
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#### J.S. Yadav, B.V. Subba Reddy, A. Srinivas Reddy

Journal of Molecular Catalysis A: Chemical 280 (2008) 219

Phosphomolybdic acid-supported silica gel as efficient and cost-effective solid acid for the benzylation of indoles with benzylic alcohols

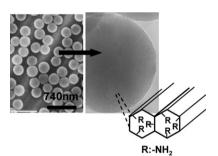




#### Tomiko M. Suzuki, Tadashi Nakamura, Keiko Fukumoto, Masami Yamamoto, Yusuke Akimoto, Kazuhisa Yano

Journal of Molecular Catalysis A: Chemical 280 (2008) 224

Direct synthesis of amino-functionalized monodispersed mesoporous silica spheres and their catalytic activity for nitroaldol condensation New amino-functionalized monodispersed mesoporous silica spheres with ordered hexagonal regularity were successfully synthesized directly by co-condensation. Evaluations of the base catalytic activity of these particles confirm their effectiveness in catalysis due to their radially aligned mesopores.



#### Jinhua Jiang, Qiuming Gao, Zhi Chen

Journal of Molecular Catalysis A: Chemical 280 (2008) 233

Gold nanocatalysts supported on protonic titanate nanotubes and titania nanocrystals

In this manuscript, we deposited Au nanoparticles on titanate nanotubes, and then converted the Au/titanate to Au/titania via an acetic acid treatment. The porosity, crystal structure and morphology of those composites have been studied by XRD, HRTEM, and low-temperature nitrogen adsorption. Both of Au/titanate and Au/titania have good performance on CO catalytic oxidation. Influence of support differences in structure and surface was discussed preliminarily.

