



Journal of Molecular Catalysis A: Chemical 275 (2007) v-xiii

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# Contents

### Articles

# Kotohiro Nomura, Takashi Atsumi, Michiya Fujiki, Junji Yamada

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Efficient ring-opening metathesis polymerization of norbornene by vanadium-alkylidenes generated *in situ* from V(NAr)Cl<sub>2</sub>(L) (L: ketimide, aryloxo)



# Lu-Ning Huang, Xin-Ping Hui, Zhi-Ce Chen, Chao Yin, Peng-Fei Xu, Xiao-Xia Yu, Shao-Yi Cheng

A chiral  $\beta$ -hydroxy amide was synthesized from L-phenylalanine and successfully grafted onto amorphous silica gel. Asymmetric addition of phenylacetylene to aldehydes was catalyzed by silica-immobilized titanium(IV) complex of  $\beta$ -hydroxy amides with good enantioselectivities (up to 81% ee). After readily recoverable procedure, the ligand could be reused several times without serious loss of enantioselectivity.

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Enantioselective addition of phenylacetylene to aldehydes catalyzed by silica-immobilized titanium (IV) complex of  $\beta$ -hydroxyamide



#### Nikunj Bhatt, Anjali Patel, Parasuraman Selvam, Kalpesh Sidhpuria

Journal of Molecular Catalysis A: Chemical 275 (2007) 14

Fresh and calcined supported 12-tungstosilicicacid: Synthesis, characterization and application to some acid catalyzed reactions 12-Tungstosilicicacid (TSA) supported onto neutral alumina has been synthesized and characterized by various physicochemical techniques and used as solid acid catalyst for carrying out acid catalyzed reactions. The results were compared with 12-tungstosilicicacid supported onto hydrous zirconia in order to see the effect of nature of support.

tert-butylation of phenol.



#### Mohammad A. Bigdeli, Majid M. Heravi, Gholam Hossein Mahdavinia

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Silica supported perchloric acid ( $HClO_4$ -SiO<sub>2</sub>): A mild, reusable and highly efficient heterogeneous catalyst for the synthesis of 14-aryl or alkyl-14-*H*-dibenzo[*a*,*j*]xanthenes

 $HClO_4$ -SiO<sub>2</sub> provides a simple, efficient, rapid and environmentally benign route for the synthesis of 14-aryl or alkyl-14-*H*-dibenzo[*a*,*j*]xanthenes.



#### Gonghu Li, Le Chen, Michael E. Graham, Kimberly A. Gray

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A comparison of mixed phase titania photocatalysts prepared by physical and chemical methods: The importance of the solid–solid interface Mixed phase titiana prepared by reactive magnetron sputtering demonstrated better photocatalytic activity than those prepared by other methods. The improved photoactivity is suggested to be associated with a unique distribution of charge trapping sites and a high density of solid–solid interfaces between anatase and rutile phases in the sputtered titania materials.



### Zhen Zhang, Junpeng Xing, Jing Li, Xiangguang Yang

Journal of Molecular Catalysis A: Chemical 275 (2007) 36

Investigation of "Rearrangement Step" in classical Beckmann rearrangement mechanism over solid acid by means of <sup>18</sup>O isotopic labeling

Beckmann rearrangement mechanism in gas phase and catalyzed by  $B_2O_3/\gamma$ - $Al_2O_3$  and TS-1 have been investigated by isotope labeling approach. The formed water is only partially released or there is still some interaction between the formed  $H_2O$  and the nitrilium cation. Dissociation degree ( $\alpha$ ) values for  $B_2O_3/\gamma$ - $Al_2O_3$  and TS-1 are 0.199 and 0.806 at reaction conditions, respectively.



#### Hai-Feng Zhou, Qing-Hua Fan, Yi-Yong Huang, Lei Wu, Yan-Mei He, Wei-Jun Tang, Lian-Quan Gu, Albert S.C. Chan

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Mixture of poly(ethylene glycol) and water as environmentally friendly media for efficient enantioselective transfer hydrogenation and catalyst recycling The asymmetric transfer hydrogenation of nonfunctionalized aromatic ketones catalyzed by Ru-TsDPEN catalyst was performed successfully in a mixture of poly(ethylene glycol) (PEG) and water with high activity and enantioselectivity. The unmodified catalyst could be easily recovered after extraction of the reduced product with a less polar solvent such as hexane, and was reused at least 14 times without obvious loss in enantioselectivity.



[RuCl<sub>2</sub>(*p*-cymene)]<sub>2</sub> + (1*S*, 2*S*)-TsDPEN HCOONa, 40 °C PEG/H<sub>2</sub>O



#### Ned A. Stephenson, Alexis T. Bell

Journal of Molecular Catalysis A: Chemical 275 (2007) 54

Mechanistic insights into iron porphyrin-catalyzed olefin epoxidation by hydrogen peroxide: Factors controlling activity and selectivity A summary is presented of our previous research efforts regarding the mechanistic understanding of porphyrin-catalyzed epoxidation of olefins by hydrogen peroxide. The sum of the work presents a mechanism that describes accurately the effects of alcohol, porphyrin, substrate, hydrogen peroxide, and solvent compositions and concentrations on selectivity and activity.



#### Shuhui Cai, Viorel Chihaia, Karl Sohlberg

Methane, ethane and pentane can be dehydrogenated by interaction with a  $\gamma$ -alumina surface. Several interaction configurations lead to dehydrogenation, including this two-center interaction of methane.

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Interactions of methane, ethane and pentane with the (110C) surface of  $\gamma$ -alumina



### Xue Jiang, Xiuzhi Tian, Zhiqiang Fan, Kuanjun Fang, Zhisheng Fu, Junting Xu, Qi Wang

Journal of Molecular Catalysis A: Chemical 275 (2007) 72

Control of the molecular weight distribution and tacticity in 1-hexylene polymerization catalyzed by  $\rm TiCl_4/MgCl_2-NaCl/TEA$  catalysis system

The deconvolution of the molecular weight distribution profile showed that the active center of the  $TiCl_4/MgCl_2-NaCl/TEA$  catalysis system can be controlled by the doping of  $MgCl_2$  by NaCl.



#### K.M. Parida, Sujata Mallick

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Silicotungstic acid supported zirconia: An effective catalyst for esterification reaction

The esterification of acetic acid with various alcohols is an electrophilic substitution reaction, catalysed by strong Br\u03c6nsted acid sites. The influence of reaction time on the acetic acid conversion was given above using 15 wt% ZSTA as catalyst (0.025 g). A gradual rise in the conversion was seen with increase in duration of the reaction period. As seen from figure, in 4 h of reaction time, 91.5% of conversion is obtained, where as at the end of 5 h only 92% of the reaction is complete.



# C. Mahendiran, P. Sangeetha, P. Vijayan, S.J. Sardhar Basha, K. Shanthi

substituted MCM-41 molecular sieves

Journal of Molecular Catalysis A: Chemical 275 (2007) 84

Vapour phase oxidation of tetralin over Cr and Fe

Vapour phase oxidation of tetralin to 1-tetralone using molecular oxygen is reported for the first time on Cr and Fe substituted MCM-41 molecular sieves. The reaction is considered to occur in two steps: oxidation of tetralin to tetralol and oxidation of the latter to 1-tetralone, with the former process occurring over  $Cr^{3+}$  and the latter over  $Cr^{6+}$ .



# Jonathan D. Webb, Daniel J. Harrison, David W. Norman, Johanna M. Blacquiere, Christopher M. Vogels, Andreas Decken, Craig G. Bates, D. Venkataraman, R. Thomas Baker, Stephen A. Westcott Journal of Molecular Catalysis A: Chemical 275 HB(OR)<sub>2</sub> HB(OR)<sub>2</sub> (2007) 91 B(OR)<sub>2</sub> B(OR)2 5 mol% [Rh] 5 mol% [lr] Metal catalysed hydroboration of vinyl sulfides, sulfoxides, sulfones, and sulfonates Serge A. Mitchenko, Tatyana V. Krasnyakova, Regina S. Mitchenko, Alexander N. Korduban

Journal of Molecular Catalysis A: Chemical 275 (2007) 101

Acetylene catalytic hydrochlorination over powder catalyst prepared by pre-milling of K<sub>2</sub>PtCl<sub>4</sub> salt



#### Najmodin Azizi, Lalleh Torkian, Mohammad R. Saidi

Journal of Molecular Catalysis A: Chemical 275 (2007) 109

Highly efficient synthesis of bis(indolyl)methanes in water





► [MnPCIO,]

#### Dorota Rutkowska-Zbik, Malgorzata Witko

Journal of Molecular Catalysis A: Chemical 275 (2007) 113

From activation of dioxygen to formation of high-valent oxo species: Ab initio DFT studies



[MnPCIO<sub>2</sub>H]

[MnPCIO]H<sub>2</sub>O

CO+H2



ligands. The mechanism of the reaction for the hydroformylation of 3β-acetoxycholest-4-ene was

Andreia F. Peixoto, Mariette M. Pereira, Artur M.S. Silva, Cláudia M. Foca, J. Carles Bayón, Maria José S.M. Moreno, Ana Matos Beja, José A. Paixão, Manuela Ramos Silva

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Hydroformylation of hindered double bonds of natural products with rhodium catalysts: The effect of 3-acetoxy substituent

#### Ikuo Atake, Kazufumi Nishida, Dalin Li, Tetsuya Shishido, Yasunori Oumi, Tsuneji Sano, Katsuomi Takehira

Journal of Molecular Catalysis A: Chemical 275 (2007) 130

Catalytic behavior of ternary Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> systems prepared by homogeneous precipitation in water-gas shift reaction

Ternary Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts were prepared by urea-assisted homogeneous precipitation and the precipitation procedures were studied. Aurichalcite as the catalyst precursor played an important role in the activity for the water-gas shift reaction.

investigated, through the hydroformylation of (1R)-(-)-myrtenyl acetate as a cyclic allylic acetate model.



[MnPCIO\_H]

# Ahmad M. Al-Ajlouni, Tariq M. Daiafla, Mohammad El-Khateeb

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New nitrophenyl-substituted polyperoxotungstate catalyst: A more active and selective for the oxidation of sulfides by hydrogen peroxide





#### Atul Manvar, Pravin Bochiya, Vijay Virsodia, Rupesh Khunt, Anamik Shah

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Microwave-assisted and  $Zn[L-proline]_2$  catalyzed tandem cyclization under solvent free conditions: Rapid synthesis of chromeno[4,3-*c*]pyrazol-4-ones



#### Eliška Leitmannová, Libor Červený

Journal of Molecular Catalysis A: Chemical 275 (2007) 153

Sorbic alcohol hydrogenation

Sorbic alcohol hydrogenation was carried out in homogeneous, two-phase and heterogeneous arrangements. The influence of reaction condition to the reaction rate and selectivity was observed. The highest selectivity was reached using ethylene glycol as a solvent and in two-phase arrangement where ethylene glycol was as catalyst phase used.



# H. Hentit, K. Bachari, M.S. Ouali, M. Womes, B. Benaichouba, J.C. Jumas

Alkylation of benzene and other aromatics by benzyl chloride to diphenylmethane over iron-containing aluminophosphate molecular sieves FAPO-5, and FAPO-11 has been investigated.

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Alkylation of benzene and other aromatics by benzyl chloride over iron-containing aluminophosphate molecular sieves





# Benjaram M. Reddy, Gode Thrimurthulu, Pranjal Saikia, Pankaj Bharali

Journal of Molecular Catalysis A: Chemical 275 (2007) 167

Silica supported ceria and ceria-zirconia nanocomposite oxides for selective dehydration of 4methylpentan-2-ol





#### Baskaran Rajesh, Natarajan Sasirekha, Yu-Wen Chen

Journal of Molecular Catalysis A: Chemical 275 (2007) 174

Physicochemical and catalytic properties of Fe-P ultrafine amorphous catalysts

Fe-P ultrafine amorphous alloy particles were prepared using chemical reduction method and characterized by XRD, TEM, N<sub>2</sub> sorption, electron diffraction, and XPS. The structure, morphology, and composition of Fe-P nanoalloys have been significantly influenced by the iron precursor and

the type of solvent used.

#### Qing Sun, Yuchuan Fu, Haixia Yang, Aline Auroux, Jianyi Shen

Journal of Molecular Catalysis A: Chemical 275 (2007) 183

Dehydration of methanol to dimethyl ether over Nb2O5 and NbOPO4 catalysts: Microcalorimetric and FT-IR studies

The probe molecules (NH<sub>3</sub>, methanol, H<sub>2</sub>O and dimethyl ether) used in this work were adsorbed more strongly on niobium phosphate (NbOPO $_{4}$ ) than on Nb<sub>2</sub>O<sub>5</sub> because of the stronger acidity of NbOPO<sub>4</sub>. In the reaction of methanol dehydration, although Nb<sub>2</sub>O<sub>5</sub> and NbOPO<sub>4</sub> were not as active as a H-ZSM-5 zeolite, they exhibited 100% selectivity to the DME product and a good stability of the activity in the temperature range relevant to the reaction (453-573 K), without coke formation.



20 nm

# Wenzhen Zhang, Ping Liu, Kun Jin, Ren He

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Synthesis, characterization and catalytic activity for ring-closing metathesis of ruthenium benzylidene complexes bearing N-heterocyclic carbene and bidentate phosphino-carboxylate ligands

The synthesis, characterization, and ring-closing metathesis (RCM) activity of new ruthenium benzylidene complexes bearing N-heterocyclic carbene and chelating phosphino-carboxylate ligands are presented. Catalysts featuring a five-membered or rigid six-membered chelating ring proved to exhibit enhanced stability and high catalytic efficiency toward the RCM reactions of diethyl diallylmalonate and diallylmalononitrile, especially at increased temperature.



Compared with Pt species, Pd species are easy to intercalate into the lattice of  $TiO_2$ , producing a

#### Hsin-Hung Ou, Shang-Lien Lo

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significantly negative effect on TCE degradation. Meanwhile, Pt had no influence on the selectivity toward DCAC and phosgene whereas the selectivity toward phosgene in the presence of Pd was enhanced owing to the easy cleavage of the C-C bond within hydrocarbon radicals.





Amélia P. Rauter, Tânia Almeida, Nuno M. Xavier, Filipa Siopa, Ana I. Vicente, Susana D. Lucas, João P. Marques, Fernando Ramôa Ribeiro, Michel Guisnet, Maria J. Ferreira

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Acid zeolites as efficient catalysts for *O*- and *S*-glycosylation

The zeolites HY, HBEA and HZSM-5 were investigated for glycosylation using two glycosyl donor types: *N*-acetylgalactosamine and a glycal. Regioselectivity for the furanoside form occurred in the Fischer glycosidation with all the catalysts. They also proved to be effective in transforming a benzyl-protected glycal into Ferrier products. Their efficiency depended mainly upon their Brönsted acid sites concentration and hydrophilicity for both reactions.





# P. Madhusudhan Rao, P. Goldberg-Oppenheimer, S. Kababya, S. Vega, M.V. Landau

Journal of Molecular Catalysis A: Chemical 275 (2007) 214

Proton enriched high-surface-area cesium salt of phosphotungstic heteropolyacid with enhanced catalytic activity fabricated by nanocasting strategy



# Petro Lahtinen, Jahir Uddin Ahmad, Elina Lankinen, Petri Pihko, Markku Leskelä, Timo Repo

Journal of Molecular Catalysis A: Chemical 275 (2007) 228

Organocatalyzed oxidation of alcohols to aldehydes with molecular oxygen

The first direct oxidation of benzylic alcohols to aldehydes with a 9,10-diaminophenanthrene organocatalyst using molecular oxygen as terminal oxidant is described. Transition metal ions increase the catalytic activity of the reaction significantly. Up to 80% conversion from alcohol to aldehyde were observed in organocatalytic reaction and complete conversions in the presence of iron and copper ions.



# C. Bolfa, A. Zoleo, A.S. Sassi, A.L. Maniero, D. Pears, K. Jerabek, B. Corain

Journal of Molecular Catalysis A: Chemical 275 (2007) 233

Cross-linked poly-vinyl polymers versus polyureas as designed supports for catalytically active  $M^0$  nanoclusters. Part I. Nanometer scale structure of the polyurea support  $EnCat^{\rm TM}\,40$ 





3470 3480

3430 3440 3450 3460

3400 3410 3420 3430 3440 3450 3460 3470 3480 3400 3410 3420

xii

# Walt Partenheimer

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Comments on the paper "Low-bromide containing MC catalyst for the autoxidation of *para*-xylene" by B. Saha and J.H. Espenson [J. Mol. Catal. A 271 (2007) 1–5]

# Rajendra Srivastava

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Corrigendum to "An efficient, eco-friendly process for aldol and Michael reactions of trimethylsilyl enolate over organic base-functionalized SBA-15 catalysts" [J. Mol. Catal. A: Chem. 264 (2007) 146–152]