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## Journal of Molecular Catalysis A: Chemical

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## Contents

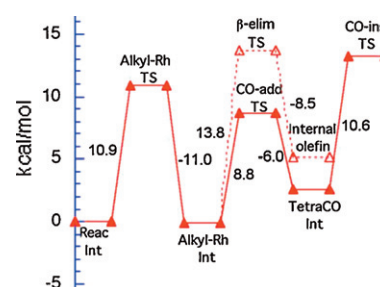
## Articles

**Raffaello Lazzaroni, Roberta Settambolo,  
Giuliano Alagona, Caterina Ghio**

*Journal of Molecular Catalysis A: Chemical 356 (2012) 1*

High linear regioselectivity in the rhodium-catalyzed hydro(deuterio)formylation of 3,4,4-trimethylpent-1-ene: The role of  $\beta$ -hydride elimination

► Regioselectivity is in favor of linear aldehydes for  $\alpha$ -methylsubstituted alkenes at rt. ► Deuterioformylation runs put forward  $\beta$ -elimination for branched Rh-alkyl intermediates. ► Theoretical results on the full catalytic cycle elucidate why and where this occurs.

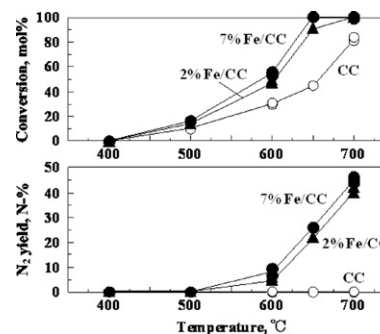


**Tetsuya Matsuyama, Naoto Tsubouchi,  
Yasuo Ohtsuka**

*Journal of Molecular Catalysis A: Chemical 356 (2012) 14*

Catalytic decomposition of nitrogen-containing heterocyclic compounds with highly dispersed iron nanoparticles on carbons

► Fe catalysts supported on carbons have been utilized to decompose the N in pyrrole or pyridine to  $N_2$ . ► The catalyst is mainly prepared by heating FeOOH precipitated onto powdery cellulose. ► Nanoscale iron particles promote  $N_2$  formation from pyrrole or pyridine at temperatures of  $>500^\circ\text{C}$ . ►  $N_2$  yields are 40–45% after the almost complete decomposition of these heterocyclic N-compounds. ► The activity of Fe catalyst for  $N_2$  formation is very sensitive to the iron particle size.

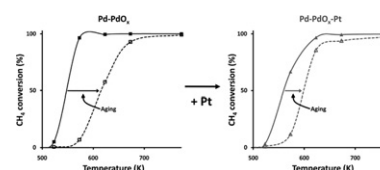


**Niko M. Kinnunen, Janne T. Hirvi, Mika Suvanto,  
Tapani A. Pakkanen**

*Journal of Molecular Catalysis A: Chemical 356 (2012) 20*

Methane combustion activity of Pd–PdO<sub>x</sub>–Pt/Al<sub>2</sub>O<sub>3</sub> catalyst: The role of platinum promoter

► Addition of Pt improves aging durability of the Pd–PdO<sub>x</sub> catalyst. ► Active phase of the catalysts consists of metallic (M) and metal oxide (MO<sub>x</sub>) sites. ► The M/MO<sub>x</sub> ratio corresponds to CH<sub>4</sub> combustion activity. ► The function of Pt promoter is to increase number of metallic sites on the active phase.

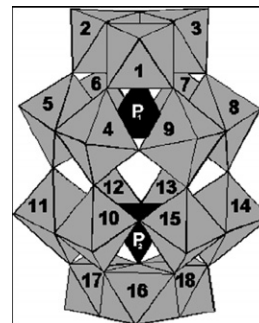


**Leila Dermeche, Nassima Salhi, Smain Hocine, René Thouvenot, Chérifa Rabia**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 29

Effective Dawson type polyoxometallate catalysts for methanol oxidation

►  $K_6P_2W_{18-x}Mo_xO_{62}$  ( $x = 0, 5, 6$ ) and  $\alpha 1$  and  $\alpha 2$ - $K_7P_2W_{12}Mo_5VO_{62}$ , Dawson polyoxometalates. ► Catalysts for methanol oxidation. ► The major products are formaldehyde, methyl formate, dimethylether and dimethoxymethane. ► The reaction products depend on the choice of elements constituting the heteropolyanion. ► Dawson heteropolyanions are as good design to guide the methanol oxidation.

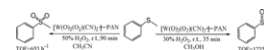


**Siva Prasad Das, Jeena Jyoti Boruah, Niharika Sharma, Nashreen S. Islam**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 36

New polymer-immobilized peroxotungsten compound as an efficient catalyst for selective and mild oxidation of sulfides by hydrogen peroxide

► A new W(VI) catalyst has been developed by incorporating peroxotungsten(VI) species into poly(acrylonitrile) matrix. ► The catalyst efficiently mediates selective oxidation of various sulfides and dibenzothiophene by  $H_2O_2$  to sulfoxide or sulfone. ► The oxidations take place under mild conditions with high TOF. ► The catalyst can be recovered and reused at least for seven reaction cycles with consistent activity and selectivity.

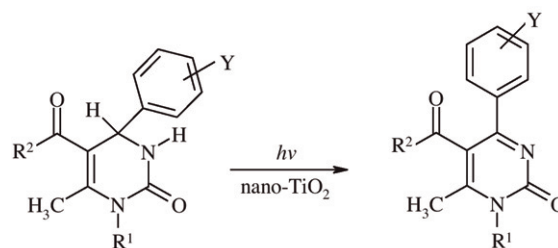


**Hamid R. Memarain, Mahnaz Ranjbar**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 46

Substituent effect in photocatalytic oxidation of 2-oxo-1,2,3,4-tetrahydropyrimidines using  $TiO_2$  nanoparticles

► Photooxidation of 2-oxo-1,2,3,4-tetrahydropyrimidines was investigated by  $TiO_2$  anatase nanoparticles. ► The nature of the heterocyclic ring substituents influences the rate of reaction. ► Drastic effect is observed by the substitution on the N1 of the heterocyclic ring. ► Experimental and theoretical results support the proposed electron-transfer mechanism. ► The nature of solvent affects the rate of reaction.

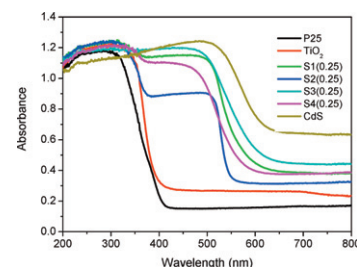


**Jian-wen Shi, Xiaoxia Yan, Hao-jie Cui, Xu Zong, Ming-Lai Fu, Shaohua Chen, Lianzhou Wang**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 53

Low-temperature synthesis of  $CdS/TiO_2$  composite photocatalysts: Influence of synthetic procedure on photocatalytic activity under visible light

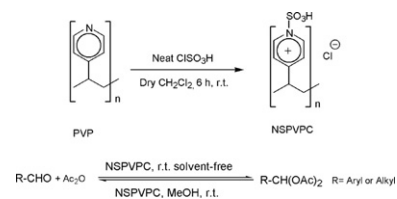
►  $CdS/TiO_2$  composite was prepared at a considerably low temperature ( $180^\circ C$ ). ► Four different procedures were used to synthesize  $CdS/TiO_2$  composite. ► The absorption edge of  $TiO_2$  was extended to 550 nm due to the addition of  $CdS$ . ► The resulting  $CdS/TiO_2$  showed high photocatalytic activity under visible light.



**Farhad Shirini, Omid Goli Jolodar***Journal of Molecular Catalysis A: Chemical* 356 (2012) 61

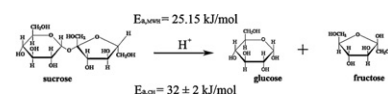
Introduction of *N*-sulfonic acid poly(4-vinylpyridinum) chloride as an efficient and reusable catalyst for the chemoselective 1,1-diacetate protection and deprotection of aldehydes

► Synthesis of *N*-sulfonic acid poly(4-vinylpyridinum) chloride (NSPVPVC). ► Characterization and application of NSPVPVC for the acylation of aldehydes and deprotection of the obtained 1,1-diacetates. ► Catalysis under solvent-free conditions. ► Heterogeneous catalysis and recyclability of the catalyst.

**Borivoj K. Adnadjevic, Jelena D. Jovanovic***Journal of Molecular Catalysis A: Chemical* 356 (2012) 70

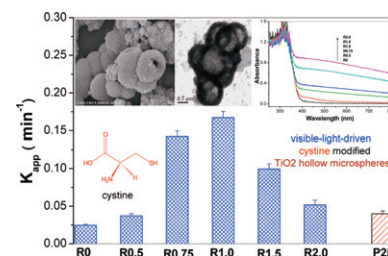
A comparative kinetics study on the isothermal heterogeneous acid-catalyzed hydrolysis of sucrose under conventional and microwave heating

► The sucrose's hydrolysis rate is 5–10 times higher for microwave heating (MWH). ► The MWH did not change the kinetics model of heterogeneous sucrose hydrolysis. ► The kinetics parameters are lower for MWH than for the conventional heating (CH). ► The increased rate of hydrolysis is not a consequence of overheating of MWH.

**Kangle Lv, Juncheng Hu, Xianghong Li, Mei Li***Journal of Molecular Catalysis A: Chemical* 356 (2012) 78

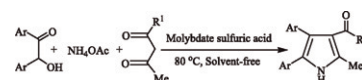
Cysteine modified anatase  $\text{TiO}_2$  hollow microspheres with enhanced visible-light-driven photocatalytic activity

► Visible-light-driven  $\text{TiO}_2$  hollow microspheres were prepared by cysteine modification. ► C, N and S elements were doped into the lattices of  $\text{TiO}_2$  hollow microspheres. ► Reasons for the enhanced visible-light-driven photocatalytic activity are discussed. ► This method is simple, cost-effective, and environmental friendly.

**Fatemeh Tamaddon, Mahnaz Farahi, Bahador Karami***Journal of Molecular Catalysis A: Chemical* 356 (2012) 85

Molybdate sulfuric acid as a reusable solid catalyst in the synthesis of 2,3,4,5-tetrasubstituted pyrroles via a new one-pot [2+2+1] strategy

► MSA catalyzes efficiently the one-pot [2+2+1] strategy for the synthesis of substituted pyrroles. ► The yield of MSA-catalyzed reaction of 1,3-dicarbonyls,  $\text{NH}_4\text{OAc}$ , and benzoin is high. ► This heterogeneous solid acid catalyst is recyclable. ► Electron-deficient benzoin reacted much faster than the others in the presence of MSA.

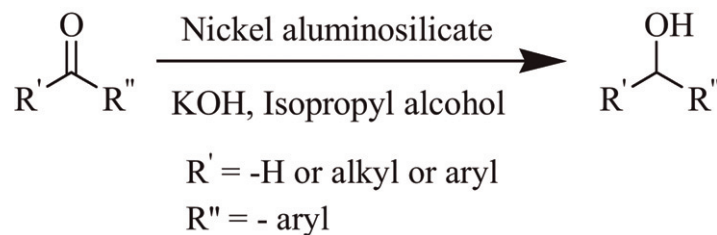


**N. Neelakandeswari, G. Sangami,  
P. Emayavaramban, S. Ganesh Babu,  
R. Karvembu, N. Dharmaraj**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 90

Preparation and characterization of nickel aluminosilicate nanocomposites for transfer hydrogenation of carbonyl compounds

► Nickel aluminosilicate nanocomposites were prepared by sol-gel technique and characterized by various physicochemical techniques. ► Transfer hydrogenation of carbonyl compounds were carried out using the prepared catalyst. ► 2-Chloro-3-formyl quinoline and its derivatives were reduced to their corresponding alcohols in excellent yield.

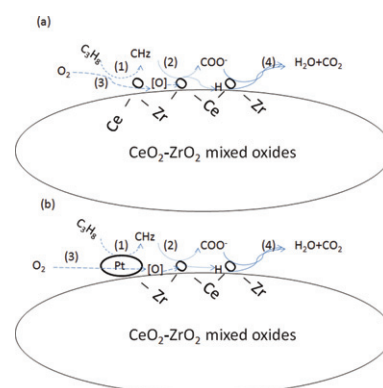


**Bin Wang, Xiaodong Wu, Rui Ran,  
Zhichun Si, Duan Weng**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 100

IR characterization of propane oxidation on Pt/CeO<sub>2</sub>-ZrO<sub>2</sub>: The reaction mechanism and the role of Pt

► The addition of Pt increases propane oxidation activity at the low temperature. ► The oxidation of Ce<sup>3+</sup> and regeneration of Ce<sup>4+</sup> is important to the oxidation reaction. ► Bidentate carbonate species are thought to be the intermediate of the oxidation reaction. ► The desorption of products is mainly related to CeO<sub>2</sub>-ZrO<sub>2</sub> support.

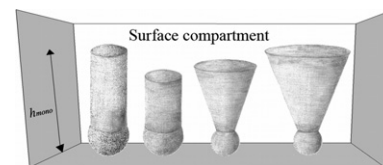


**M. Soledade C.S. Santos, Ester F.G. Barbosa**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 106

Silver (I) activated quaternization of tertiary amines by alkyl iodides: Overall analysis coupling homogeneous and heterogeneous processes

► Experimental data for new systems substantiated model previously proposed. ► Stereochemical and electronic effects governing solution and surface processes were scrutinized. ► Molecular level analysis afforded the definition of unitary superficial reaction compartments. ► "Volumetric surface rate constants" allowed the direct comparison of solution and surface rates.

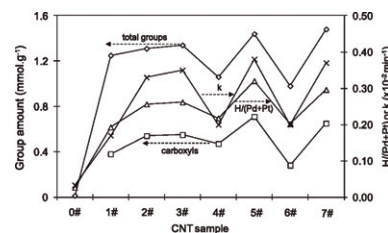


**Jiuling Chen, Qinghai Chen, Qing Ma,  
Yongdan Li, Zhonghua Zhu**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 114

Chemical treatment of CNTs in acidic KMnO<sub>4</sub> solution and promoting effects on the corresponding Pd-Pt/CNTs catalyst

► Treatment of CNTs in KMnO<sub>4</sub> was investigated on formation of surface groups. ► Relationship between treatment conditions and formed groups was investigated. ► Promoting effects on Pd-Pt/CNTs catalyst was illustrated.

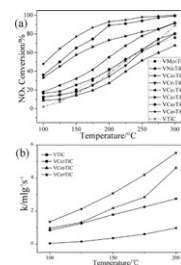


**Qian Li, Xiaoxu Hou, Hangsheng Yang,  
Zhaoxia Ma, Junwei Zheng, Fu Liu,  
Xiaobin Zhang, Zhongyong Yuan**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 121

Promotional effect of  $\text{CeO}_x$  for NO reduction over  $\text{V}_2\text{O}_5/\text{TiO}_2$ -carbon nanotube composites

► A series of  $\text{V}_2\text{O}_5\text{-CeO}_x/\text{TiO}_2\text{-CNTs}$  catalysts were synthesized by sol-gel. ► A catalytic promotional effect was observed by adding  $\text{CeO}_x$  into  $\text{V}_2\text{O}_5/\text{TiO}_2\text{-CNTs}$ . ► The reducibility, acidity, chemisorbed oxygen increased with introduction of  $\text{CeO}_x$ .

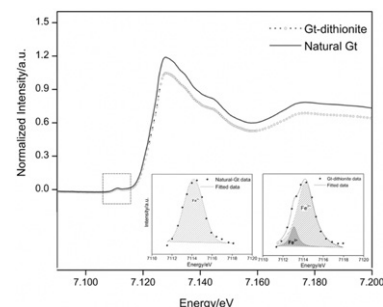


**Anelise L. de Abreu, Iara R. Guimarães,  
Alexandre dos S. Anastácio, Mário C. Guerreiro**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 128

Natural goethite reduced with dithionite: Evaluation of the reduction process by XANES and Mössbauer spectroscopy and application of the catalyst in the oxidation of model organic compounds

► Goethite-dithionite: a new catalyst for oxidation using a Fenton like system. ► Dithionite as a cheap reducing reagent for iron oxide activation. ► The study by XANES showed iron in octahedral and tetrahedral structure. ► The reduction is related to the electron transfer active radicals to the goethite surface. ► Dithionite reduced goethite and  $\text{H}_2\text{O}_2$  for oxidation of N and S containing compounds.

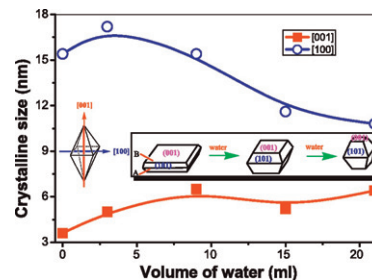


**Yang Zheng, Kangle Lv, Zhouyou Wang,  
Kejian Deng, Mei Li**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 137

Microwave-assisted rapid synthesis of anatase  $\text{TiO}_2$  nanocrystals with exposed  $\{0\ 0\ 1\}$  facets

► High-energy  $\text{TiO}_2$  nanocrystals were rapidly synthesized at  $200^{\circ}\text{C}$  for only 30 min. ► The percentage of exposed  $\{0\ 0\ 1\}$  facets is tunable. ► Crystal planes and surface chemistry are important on photo-activity of  $\text{TiO}_2$ .

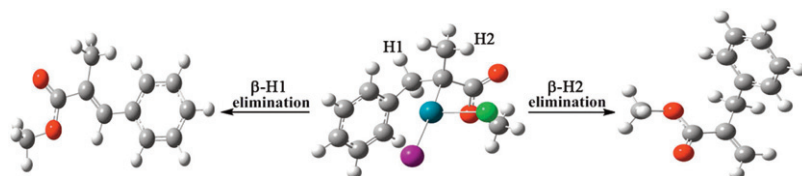


**Zorica D. Petrović, Vladimir P. Petrović,  
Dušica Simijonović, Svetlana Marković**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 144

Stereoselective homogeneous catalytic arylation of methyl methacrylate: Experimental and computational study

► Catalytic systems  $\text{trans-[PdCl}_2(\text{DEA})_2]/\text{DEA}$  or  $\text{[DEA][HAc]}$  provide homogeneous catalysis. ► Good regioselectivity and excellent stereoselectivity are achieved. ► DFT study showed that  $\beta$ -hydride elimination is key step for selectivity. ► In the first Heck cycle, internal  $E$ -olefin is the only stereoisomer. ► In the second cycle, double arylated product is  $Z$ -olefin.

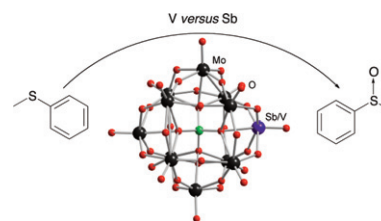


**Hila Goldberg, Devesh Kumar, G. Narahari Sastry, Gregory Leitus, Ronny Neumann**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 152

An antimony(V) substituted Keggin heteropolyacid,  $H_4PSbMo_{11}O_{40}$ : Why is its catalytic activity in oxidation reactions so different from that of  $H_4PVMo_{11}O_{40}$ ?

► An antimony(V) substituted phosphomolybdic acid was prepared and characterized. ► Different reactivity was expected versus known analogous vanadium substituted compound. ► DFT calculations explain the difference in the catalytic activity.

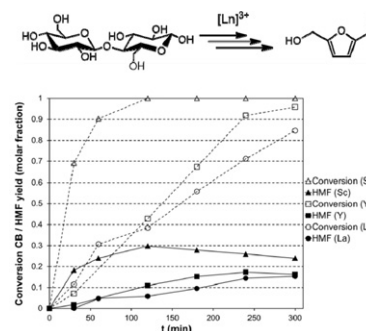


**Klaus Beckerle, Jun Okuda**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 158

Conversion of glucose and cellobiose into 5-hydroxymethylfurfural (HMF) by rare earth metal salts in *N,N'*-dimethylacetamide (DMA)

► Rare earth metal chlorides can be applied for the dehydration of carbohydrates in DMA. ► Scandium is considerably more active than yttrium or lanthanum. ► Data suggest a mechanism involving the transformation of glucose into fructose. ► Cellobiose can be transformed into HMF in a one-pot approach.

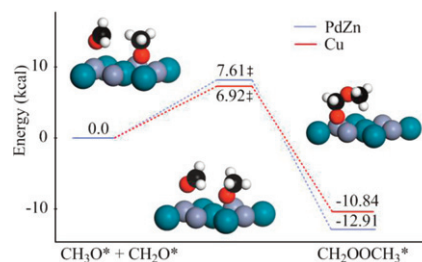


**Sen Lin, Daiqian Xie, Hua Guo**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 165

First-principles study of the methyl formate pathway of methanol steam reforming on PdZn(1 1 1) with comparison to Cu(1 1 1)

► Methyl formate can be formed between formaldehyde and methoxyl on PdZn(1 1 1). ► Methyl formate plays a minor role in methanol steam reforming (MSR) process. ► Methyl formate pathway shares many similarities with the same process on Cu(1 1 1). ► The calculated mechanism sheds valuable light on designing catalysts for MSR.



**Zhenping Qu, Shijin Shen, Dan Chen, Yi Wang**

*Journal of Molecular Catalysis A: Chemical* 356 (2012) 171

Highly active Ag/SBA-15 catalyst using post-grafting method for formaldehyde oxidation

► Highly active Ag/SBA-15 catalyst using post-grafting method for HCHO oxidation. ► HCHO can be completely oxidized into  $CO_2$  and  $H_2O$  at  $100^\circ C$  on the novel catalyst. ► Appropriate adsorption intensity between HCHO and silver sites was necessary. ► Silver particles highly dispersed on SBA-15 were active for HCHO oxidation. ► The formed intermediates can be easily activated on smaller silver particles.

