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# Journal of Molecular Catalysis A: Chemical

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# **Contents**

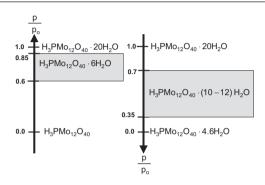
### Articles

#### Anna Micek-Ilnicka

Journal of Molecular Catalysis A: Chemical 308 (2009) 1

The role of water in the catalysis on solid heteropolyacids

The review surveys the structure of heteropolyacid (HPA) hydrates and the physicochemical properties of HPA-water system. The catalytic part of the paper includes following topics: the role of water as a substrate (hydration of olefins), product (dehydration of alcohols) and as water formally not participating in the catalytic reaction (etherification).

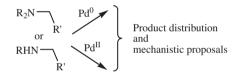


#### Jacques Muzart

Journal of Molecular Catalysis A: Chemical 308 (2009) 15

On the behavior of amines in the presence of  $Pd^{\scriptscriptstyle 0}$  and  $Pd^{\scriptscriptstyle 1}$  species

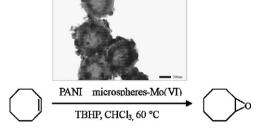
A review on the palladium-mediated intrinsic reactions of amines having hydrogens in α-position is presented.



#### Hangjun Ding, Ge Wang, Mu Yang, Yi Luan, Yingnan Wang, Xingxiong Yao

Journal of Molecular Catalysis A: Chemical 308 (2009) 25

Novel sea urchin-like polyaniline microspheressupported molybdenum catalyst: Preparation, characteristic and functionality By using sea urchin-like PANI hollow microspheres microspheres as support, a novel polymer-supported molybdenum catalyst was successfully produced. This catalyst was efficiently applied to the epoxidation of wide range of linear and cyclic alkenes. The special micro/ nanoscale spherical morphology played an important role in the enhancement of catalytic activity.

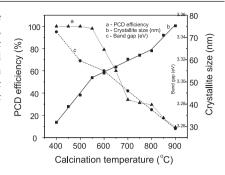


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#### S.K. Pardeshi, A.B. Patil

Journal of Molecular Catalysis A: Chemical 308 (2009) 32

Effect of morphology and crystallite size on solar photocatalytic activity of zinc oxide synthesized by solution free mechanochemical method Zinc oxide crystallites were synthesized by solution free mechanochemical method and then characterized by XRD, SEM, EDXS, FT-IR and UV-Visible spectrophotometer. Zinc oxide formed by same crystallite growth rate showed identical photocatalytic activity. Low calcination temperature, smaller particle size of zinc oxide and basic pH of suspension were favorable for photocatalytic degradation of resorcinol.



Veronica Caballero, Felipa M. Bautista, Juan Manuel Campelo, Diego Luna, Rafael Luque, Jose Maria Marinas, Antonio Angel Romero, Isabel Romero, Montserrat Rodríguez, Isabel Serrano, Jose Miguel Hidalgo, Antoni Llobet

Journal of Molecular Catalysis A: Chemical 308 (2009) 41

Efficient hydrogenation of alkenes using a highly active and reusable immobilised Ru complex on  $AIPO_{\alpha}$ 

The homogeneous ruthenium complex  $[Ru^{\parallel}Cl_2(bpea)(PPh_3)]$ , where bpea = N,N-bis-(2-pyridylmethyl)ethylamine, covalently grafted on an amorphous  $AlPO_4$  support through phosphamide bonds exhibited very good activities and excellent reusabilities (up to 25 runs) in the liquid-phase hydrogenation of alkenes.

## **Debaprasad Shee, Goutam Deo**

Journal of Molecular Catalysis A: Chemical 308 (2009) 46

Adsorption and ODH reaction of alkane on sol–gel synthesized  ${\rm TiO_2-WO_3}$  supported vanadium oxide catalysts: In situ DRIFT and structure–reactivity study

 $\rm V_2O_5/90TiO_2-WO_3$  catalysts were synthesized, characterized and studied for alkane adsorption. Propane ODH reaction data were also obtained, which correlate well with characterization studies. The alkane adsorption studies suggest that ethane and propane are adsorbed through the formation of alkoxide species, which further oxidize to other readily observed surface oxygenated species.

Possible pathways for the alkane ODH reaction based on DRIFT study of ethane, and propane adsorption. R = H for ethane and R =-CH3 for propane.

#### Francesco P. Ballistreri, Cosimo G. Fortuna, Andrea Pappalardo, Gaetano A. Tomaselli, Rosa M. Toscano

Journal of Molecular Catalysis A: Chemical 308 (2009) 56

Oxidation of organic sulfides by a vanadium(5+) oxo-monoperoxo-picolinate complex: Kinetics and mechanism

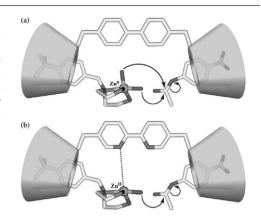
The kinetics of oxidation of p-X-benzyl phenyl- and p-Y-phenyl benzyl sulfides by V(V) oxo-monoperoxo complex  $[PicVO(O_2)]$  (Pic = picolinic acid anion) in acetonitrile at 20 °C is reported. A possible pathway for the oxygen transfer step is suggested for these reactions.

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#### Ying-Hua Zhou, Meng Zhao, Hongzhe Sun, Zong-Wan Mao, Liang-Nian Ji

Journal of Molecular Catalysis A: Chemical 308 (2009) 61

Effect of cyclodextrin dimers with bipyridyl and biphenyl linking groups on carboxyl ester hydrolysis catalyzed by zinc complex Two new cyclodextrin dimers were synthesized and applied as supramolecular catalyst precursors, in which one hydrophobic cavity is assembled with zinc complex and another hydrophobic cavity is used to capture *p*-nitrophenyl acetate. Contrast to bipyridyl-linking system, biphenyl-linking cyclodextrin system exhibits higher catalytic activity and the second-order rate constant presents exponential growth with the increasing value of pH.



#### Yinxi Zhou, Jinliang Song, Shuguang Liang, Suqin Hu, Huizhen Liu, Tao Jiang, Buxing Han

Journal of Molecular Catalysis A: Chemical 308 (2009) 68

Metal-organic frameworks as an acid catalyst for the synthesis of ethyl methyl carbonate via transesterification An efficient synthesis of ethyl methyl carbonate using metal-organic frameworks (MOFs) as acid catalyst has been realized by the transesterification of dimethyl carbonate and diethyl carbonate. It was demonstrated that MOFs can catalyze the reaction smoothly, and high yield of ethyl methyl carbonate and good selectivity could be achieved under mild conditions.

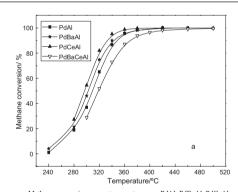
$$H_3C_{O} CH_3 + C_2H_5 C_2H_5 C_2H_5 CH_3$$

### Xiaoyu Zhang, Enyan Long, Yile Li, Lijuan Zhang, Jiaxiu Guo, Maochu Gong, Yaoqiang Chen

Journal of Molecular Catalysis A: Chemical 308 (2009) 73

The effect of CeO<sub>2</sub> and BaO on Pd catalysts used for lean-burn natural gas vehicles

 ${\rm Al_2O_3}$  supports doped by  ${\rm CeO_2}$  and/or BaO and Pd catalysts are prepared and characterized. Catalytic activities are investigated in a mixture gas simulated the exhaust emissions from leanburn natural gas vehicles (NGVs). The doping of  ${\rm CeO_2}$  or BaO alone can increase catalytic activity for methane and CO oxidation, however, the coexistence of  ${\rm CeO_2}$  and BaO causes detrimental effect to activity.



Methane conversion versus temperature over PdAl, PdBaAl, PdCeAl, PdBaCeAl catalysts in the simulated exhaust gas

# Hongquan Liu, Minghui Liang, Chao Xiao, Ning Zheng, Xuhui Feng, Yan Liu, Jinglin Xie, Yuan Wang

Journal of Molecular Catalysis A: Chemical 308 (2009) 79

An excellent Pd-based nanocomposite catalyst for the selective hydrogenation of *para*-chloronitrobenzene

 $Pd/\gamma$ -Fe<sub>2</sub>O<sub>3</sub>-PR exhibited superior selectivity to p-chloroaniline in the hydrogenation of p-chloronitrobenzene, and the catalytic hydrodechlorination of p-chloroaniline was fully suppressed.

NO<sub>2</sub>

$$H_2$$

$$Pd/\gamma - Fe_2O_3 - PR$$

$$CI$$

$$Yield: 99.2\%$$

$$NH_2$$

$$H_2$$

$$Pd/\gamma - Fe_2O_3 - PR$$

$$Vield: 99.2\%$$

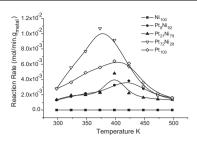
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## N.H.H. Abu Bakar, M.M. Bettahar, M. Abu Bakar, S. Monteverdi, J. Ismail, M. Alnot

Journal of Molecular Catalysis A: Chemical 308 (2009) 87

Silica supported Pt/Ni alloys prepared via co-precipitation method

Pt/Ni alloys supported on crystalline silica were prepared via co-precipitation technique using sodium borohydride as a reducing agent. The effect of Pt/Ni ratio on the hydrogenation of benzene was investigated. Pt $_{72}$ Ni $_{28}$  exhibited superior catalytic activity compared to pure Ni and pure Pt catalysts. Results indicate that alloying and Pt segregation may have contributed to this enhanced activity.

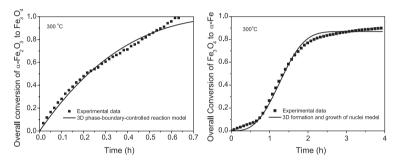


# Hong Wang, Yong Yang, Bao-Shan Wu, Jian Xu, Ming-Yue Ding, Hu-Lin Wang, Wen-Hao Fan, Hong-Wei Xiang, Yong-Wang Li

Journal of Molecular Catalysis A: Chemical 308 (2009) 96

Hydrogen reduction kinetics modeling of a precipitated iron Fischer–Tropsch catalyst

The reduction of iron FT catalyst in the temperature range of 250–350 °C was separated into two processes for the mathematical modeling. The overall reduction of  $\alpha$ -Fe $_2$ O $_3$  (PM and spm phases) to Fe $_3$ O $_4$  can be described by a three-dimensional phase-boundary-controlled reaction model, while the overall reduction of Fe $_3$ O $_4$  to  $\alpha$ -Fe follows the formation and growth of nuclei model (two-dimensional or three-dimensional).



## F. Farzaneh, M. Poorkhosravani, M. Ghandi

Journal of Molecular Catalysis A: Chemical 308 (2009) 108

Utilization of immobilized biomimetic iron complexes within nanoreactors of Al-MCM-41 as cyclohexane oxidation catalyst

The immobilized biomimetic Fe(III) complexes within nanoreactors of Al-MCM-41, characterized by powder X-ray diffraction, nitrogen adsorption—desorption, FTIR and UV—vis spectroscopy, successfully catalyze the oxidation of cyclohexane to cyclohexanol and cyclohexanone with hydrogen peroxide in refluxing acetonitrile. Fe(III) complex: [Fe(en)<sub>2</sub>Cl<sub>2</sub>]Cl, [Fe(bpy)<sub>2</sub>Cl<sub>2</sub>]Cl, [Fe(salen)Cl], [Fe(TPP)Cl], [Fe(TMC)Cl], en: ethylenediamine, bpy: 2,2′-bipyridine, salen: N,N′-bis(salicylidene)ethylenediamine), TMC: 5,7,12,14-tetramethyl-1,4,8,11 tetraazacyclotetradeca 4,6,11,13-tetraene, and TPP: meso-tetraphenylporphyrin.

#### A.G. Hardie, J.J. Dynes, L.M. Kozak, P.M. Huang

Journal of Molecular Catalysis A: Chemical 308 (2009) 114

The role of glucose in abiotic humification pathways as catalyzed by birnessite

Contents ix

#### Wenbo Kong, Weili Dai, Niu Li, Naijia Guan, Shouhe Xiang

Journal of Molecular Catalysis A: Chemical 308 (2009) 127

A one-step route to SAPO-46 using  ${
m H_3PO_3}$ -containing gel and its application as the catalyst for methanol dehydration

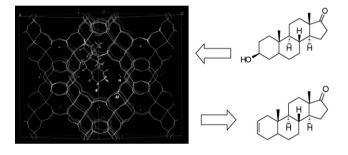
The synthesis and catalysis of SAPO-46, which is synthesized as a pure phase from a one-step route in the presence of H<sub>3</sub>PO<sub>3</sub> as the phosphorus source, have been described. It is used first as the catalyst for the formation of dimethyl ether from methanol with dimethyl ether selectivity 98.0% and higher conversion of methanol.

#### O Zoon Kwon, Se Min Park, Mee Kyung Song, Gon Seo

Journal of Molecular Catalysis A: Chemical 308 (2009) 134

Dehydration of epiandrosterone over zeolites with different pore structures and acidities

FAU zeolite with a sufficient number of acid sites showed both high conversion and selectivity for  $\Delta 2$ -olefin in the dehydration of epiandrosterone because its supercages provided enough space to form adsorbed species with tilted conformation.



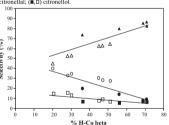
# K. Kouachi, G. Lafaye, C. Especel, O. Cherifi, P. Marécot

Journal of Molecular Catalysis A: Chemical 308 (2009) 142

Preparation of silica-supported cobalt catalysts from water-in-oil microemulsion for selective hydrogenation of citral

The performances for selective hydrogenation of citral of silica-supported Co catalysts prepared by water-in-oil (w/o) microemulsion (ME) were compared to those of previously studied Co impregnated catalysts. Above 15 wt% Co content, the selectivity to unsaturated alcohols is markedly higher on the ME catalysts compared to the impregnated ones. This result can be directly related to the higher proportion of  $\beta$  H–Co species detected by temperature-programmed desorption of hydrogen (H $_2$ -TPD) on the ME samples.

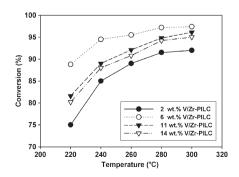
Figure. Correlation between the selectivities (at 30% citral conversion) and the percentage of the  $\beta$  H-Co species for Co-supported catalysts prepared by w/o microemulsion (ME, full caption) or impregnation (IMP, empty caption) method: (  $\bullet$ ,  $\Delta$ ) unsaturated alcohols; ( $\bullet$ ,0) citronellal; ( $\blacksquare$ ,0) citronellol.



## Kanattukara Vijayan Bineesh, Sang-Yun Kim, Balasamy Rabindran Jermy, Dae-Won Park

Journal of Molecular Catalysis A: Chemical 308 (2009) 150

Synthesis, characterization and catalytic performance of vanadia-doped delaminated zirconia-pillared montmorillonite clay for the selective catalytic oxidation of hydrogen sulfide A series of vanadia-doped zirconia-pillared clays (V/Zr-PILCs) with various amounts of vanadia were prepared and their performance for the selective catalytic oxidation of H<sub>2</sub>S was investigated in this study. V/Zr-PILCs showed better catalytic performance than as such Zr-PILC at temperatures ranging from 220 to 300 °C without any considerable SO<sub>2</sub> emission.



x Contents

#### Nabil S. Youssef, Eman El-Zahany, Ahmed M.A. El-Seidy, Alessandro Caselli, Sergio Cenini

Journal of Molecular Catalysis A: Chemical 308 (2009) 159

Synthesis and characterization of some transition metal complexes with a novel Schiff base ligand and their use as catalysts for olefin cyclopropanation The new ligand HL (1), N,2-bis(1-(2-oxo-2H-chromen-3-yl) ethylidene)hydrazinecarbothioamide was used to prepare new transition metal complexes. The catalytic activity of the copper complex, [HLCu<sub>2</sub>Cl<sub>3</sub>]Cl·H<sub>2</sub>O (2), in cyclopropanation reactions of unactivated olefins with ethyldiazoacetate (EDA) was studied. Cyclopropanes were obtained in high yield (up to 97%, TON up to 16,900).

$$R^{1} \xrightarrow{R^{2} + EDA}$$

$$R^{1} \xrightarrow{R^{2} + EDA}$$

$$R^{1} \xrightarrow{CO_{2}Et} \xrightarrow{CO_{2}Et} \xrightarrow{R^{1} \xrightarrow{CO_{2}Et}} R^{2}$$

#### B. Rama Raju, S. Sarkar, U. Chandramoulali Reddy, Anil K. Saikia

Journal of Molecular Catalysis A: Chemical 308 (2009) 169

Cerium (IV) triflate-catalyzed selective oxidation of sulfides to sulfoxides with aqueous hydrogen peroxide

$$R^{S} R' \xrightarrow{Ce(OTf)_4.xH_2O / H_2O_2} R^{O} R$$
THF /rt

# L. Gomathi Devi, B. Narasimha Murthy, S. Girish Kumar

Journal of Molecular Catalysis A: Chemical 308 (2009) 174

Photocatalytic activity of  $V^{5+}$ ,  $Mo^{6+}$  and  $Th^{4+}$  doped polycrystalline  $TiO_2$  for the degradation of chlorpyrifos under UV/solar light

 ${
m TiO}_2$  was doped with metal ions like V<sup>5+</sup>, Mo<sup>6+</sup> and Th<sup>4+</sup> in the concentration range from 0.02 to 0.1 at% and were characterized. XRD results showed that doped catalysts had only anatase phase irrespective of their nature, oxidation state, ionic size and concentration of these dopants. These photocatalysts were used for the mineralization of chlorpyrifas pesticide.

$$\begin{array}{c|c} Cl & Cl \\ & & \\ N & S \\ & & \\ Cl & O - C_2H_5 \end{array}$$

# Khadege Omari-Qadry, Khalil Hamza, Yoel Sasson, Jochanan Blum

Journal of Molecular Catalysis A: Chemical 308 (2009) 182

Liquid phase hydrodechlorination of some chlorinated aromatic nitrogen-containing heterocyclics

Chlorinated pyridine, indole, quinoline and isoquinoline derivatives are hydrodechlorinated under mild conditions by a sol–gel entrapped Pd–Rh catalyst. The reaction is associated with synergism between the two metallic nuclei.