

## Contents

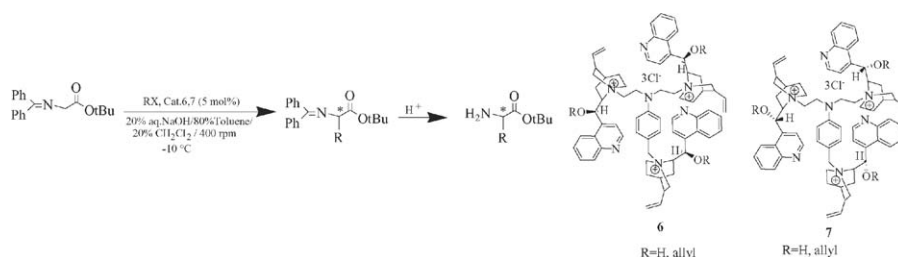
### Articles

**Ayyanar Siva, Eagambaram Murugan**

*Journal of Molecular Catalysis A: Chemical 248 (2006) 1*

New trimeric *Cinchona* alkaloid-based quaternary ammonium salts as efficient chiral phase transfer catalysts for enantioselective synthesis of  $\alpha$ -amino acids

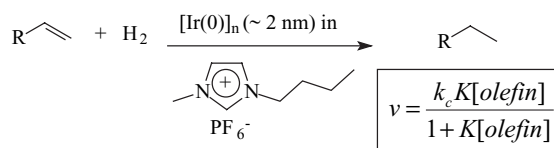
New trimeric *Cinchona* alkaloid-based quaternary ammonium salts as efficient chiral phase transfer catalysts for enantioselective synthesis of  $\alpha$ -amino acids.



**Gledison S. Fonseca, Josiel B. Domingos, Faruk Nome, Jairton Dupont**

*Journal of Molecular Catalysis A: Chemical 248 (2006) 10*

On the kinetics of iridium nanoparticles formation in ionic liquids and olefin hydrogenation

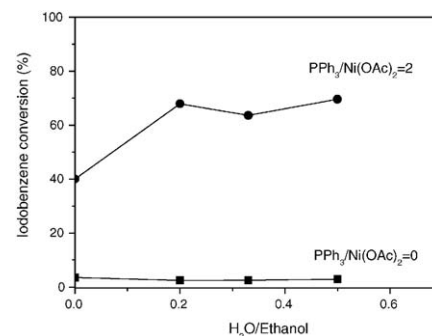


**Songyan Ma, Hongjun Wang, Kaimin Gao, Fengyu Zhao**

*Journal of Molecular Catalysis A: Chemical 248 (2006) 17*

Nickel complexes catalyzed Heck reaction of iodobenzene and methyl acrylate

Nickel appears the most promising for the replacement of palladium among the inexpensive transition metals, the effect of the addition of water is sensitive to the concentration of  $\text{PPh}_3$  and the nature of solvent in nickel-catalyzed Heck reactions.

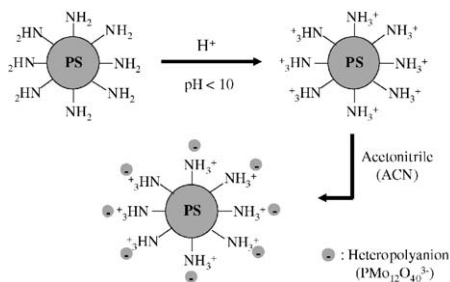


**Heesoo Kim, Ji Chul Jung, Sung Ho Yeom,  
Kwan-Young Lee, In Kyu Song**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 21

Preparation of  $H_3PMo_{12}O_{40}$  catalyst immobilized on polystyrene support and its application to the methacrolein oxidation

$H_3PMo_{12}O_{40}$  (PMo) catalyst was immobilized on the aminated polystyrene (PS) support as a charge compensating component, by taking advantage of the overall negative charge of  $[PMo_{12}O_{40}]^{3-}$ . The supported  $H_3PMo_{12}O_{40}$ -polystyrene catalyst exhibited higher catalytic performance than the unsupported catalyst in the vapor-phase oxidation of methacrolein into methacrylic acid.

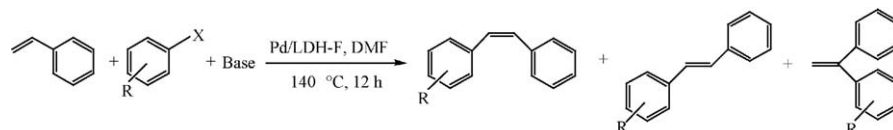


**Hao Zhou, Guang Lan Zhuo, Xuan Zhen Jiang**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 26

Heck reaction catalyzed by Pd supported on LDH-F hydroxalcite

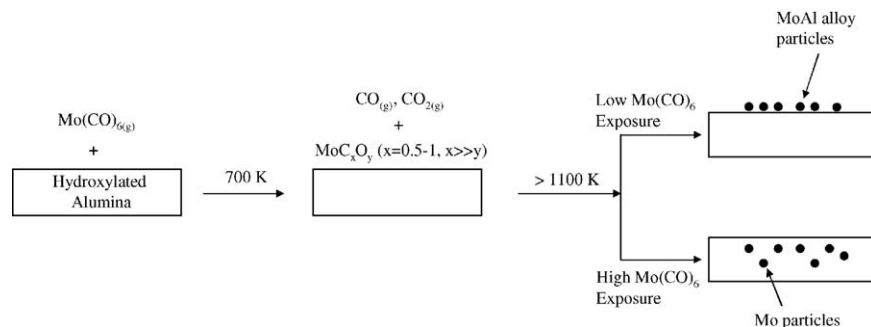
The catalyst Pd/LDH-F has been prepared and exhibits a high activity and selectivity for the first time toward the Heck reaction and reused after washing almost without loss in activity.



**Y. Wang, F. Gao, W.T. Tysoe**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 32

Interaction of molybdenum hexacarbonyl with hydroxylated alumina thin films at high temperatures: Formation and removal of surface carbides

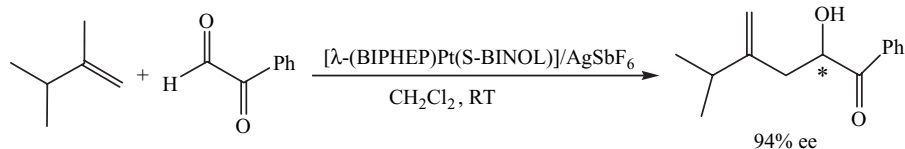


**He-Kuan Luo, Herbert Schumann**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 42

An efficient direct activation method transferring diastereopure platinum complex of BIPHEP to highly efficient Lewis acid catalyst for enantioselective carbonyl-ene reaction

An efficient direct activation method was developed to transfer diastereopure  $\lambda$ -[(BIPHEP)Pt(S-BINOL)] directly to highly selective enantiopure Lewis acid  $\lambda$ -[(BIPHEP)Pt](SbF<sub>6</sub>)<sub>2</sub> by silver hexafluoroantimonate (AgSbF<sub>6</sub>) for the enantioselective carbonyl-ene reactions between ethyl glyoxylate/phenylglyoxal and alkenes to give ee values high up to 94%.

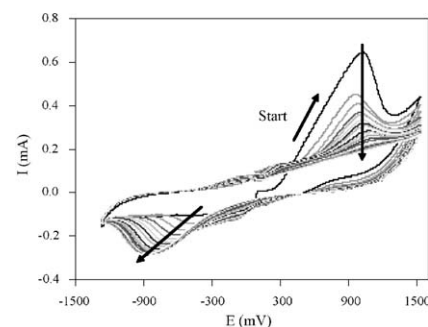


**R.H. Carvalho, F. Lemos, M.A.N.D.A. Lemos, J.M.S. Cabral, F. Ramôa Ribeiro**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 48

Electro-oxidation of phenol on zeolite/graphite composite electrodes. Part 1. Electrochemical behaviour over NaY zeolite

The oxidation of phenol was studied by cyclic voltammetry on a composite zeolite/graphite electrode. When the concentration of phenol is sufficiently low, the electrode is not deactivated by the electrochemical process. For high concentrations some of the oxidation products remain adsorbed to the zeolite, leading to a significant deactivation of the electrode material.

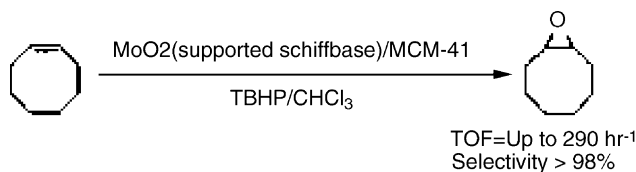


**M. Masteri-Farahani, F. Farzaneh, M. Ghandi**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 53

Synthesis and characterization of molybdenum complexes with bidentate Schiff base ligands within nanoreactors of MCM-41 as epoxidation catalysts

Incorporation of bidentate Schiff base ligands via reaction of aminopropyl modified MCM-41 with different aldehydes and ketones and subsequent treatment with  $\text{MoO}_2(\text{acac})_2$  affords a new class of heterogeneous molybdenum catalysts for epoxidation of olefins with high activity and selectivity.

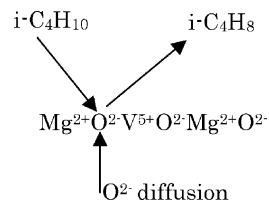


**Yusaku Takita, Qing Xia, Kayo Kikutani, Kazuya Soda, Hideaki Takami, Hiroyasu Nishiguchi, Katsutoshi Nagaoka**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 61

Anaerobic oxidation of isobutane. II. Catalysis by Mg-V complex oxides

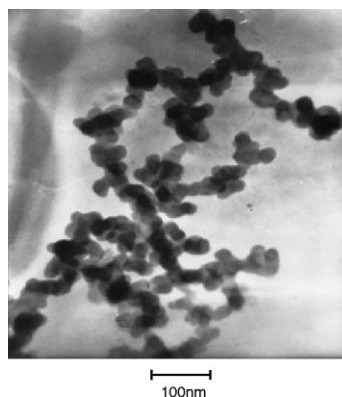
Selective oxidative dehydrogenation of isobutane is achieved over Mg-V oxides in anaerobic conditions. Highest yield of isobutene over  $\text{Mg}_2\text{V}_2\text{O}_7$  would come from the great mobility of the lattice oxygen and moderate concentration of surface active oxygen ions. Reactivity of lattice oxide ions are modified by the introduction of transition metals into the crystal lattice.



**Hongming Wang, Jingshi Xu, Ronghua Xiao, Huizong Cheng**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 70

Preparation and catalytic use of the solid acid  $\text{SO}_4^{2-}/\text{Fe}_2\text{O}_3\text{-M}_x\text{O}_y$  for the reaction of crotonaldehyde with *n*-butanol

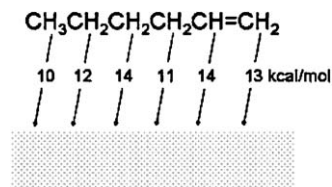


**Shuhui Cai, Karl Sohlberg**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 76

Adsorption of 1-hexene on  $\gamma$ -alumina (110C)

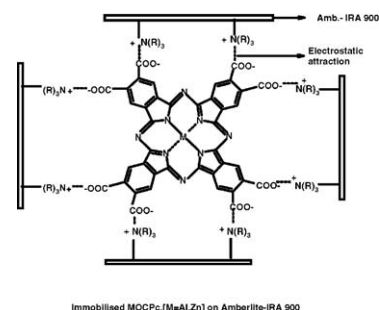
The energy barriers for abstraction of H from various positions on hexene by an oxygen-terminated alumina surface are similar, a possible explanation for the experimentally observed plethora of reaction products.

**Bolade Agboola, Kenneth I. Ozoemena, Tebello Nyokong**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 84

Comparative efficiency of immobilized non-transition metal phthalocyanine photosensitizers for the visible light transformation of chlorophenols

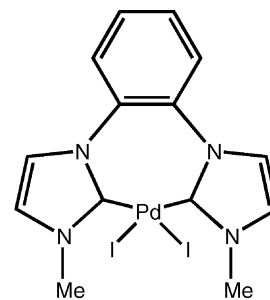
Photolysis of aqueous solutions of chlorophenols (4-chlorophenol, 2,4-dichlorophenol, 2,4,5-trichlorophenol and pentachlorophenol) in the presence of immobilized non-transition metal phthalocyanine photosensitizers onto Amberlite® results in the formation of chlorobenzoquinone derivatives.

**Cristina Tubaro, Andrea Biffis, Carlo Gonzato, Marco Zecca, Marino Basato**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 93

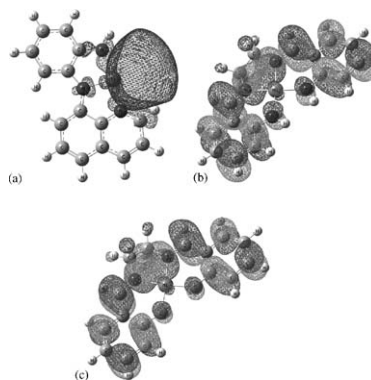
Reactivity of chelating dicarbene metal complex catalysts, I: An investigation on the Heck reaction

Chelating dicarbene ligands exhibit an inhibiting effect in the Pd-catalyzed Heck reaction of deactivated aryl bromides, which can be correlated with their ability to form inactive dimers and/or bis-chelate, tetracarbene palladium(II) derivatives.

**Morihiro Saito, Hidenobu Shiroishi, Chisato Ono, Seiji Tsuzuki, Tatsuhiko Okada, Yoshiharu Uchimoto**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 99

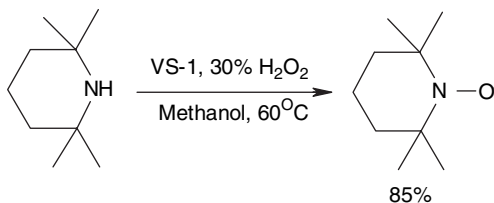
Influence of ligand structures on methanol electro-oxidation by mixed catalysts based on platinum and organic metal complexes for DMFC



**Prodeep Phukan, R.S. Khisti, A. Sudalai**

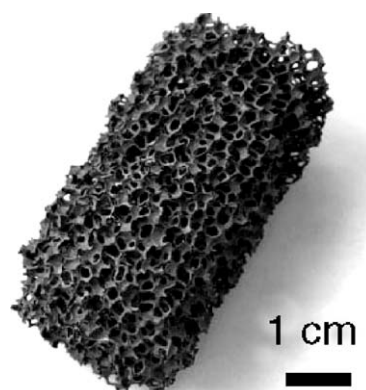
*Journal of Molecular Catalysis A: Chemical* 248 (2006) 109

Green protocol for the synthesis of N-oxides from secondary amines using vanadium silicate molecular sieve catalyst


**Gauthier Winé, Jean-Philippe Tessonnier,  
Séverinne Rigolet, Claire Marichal,  
Marc-Jacques Ledoux, Cuong Pham-Huu**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 113

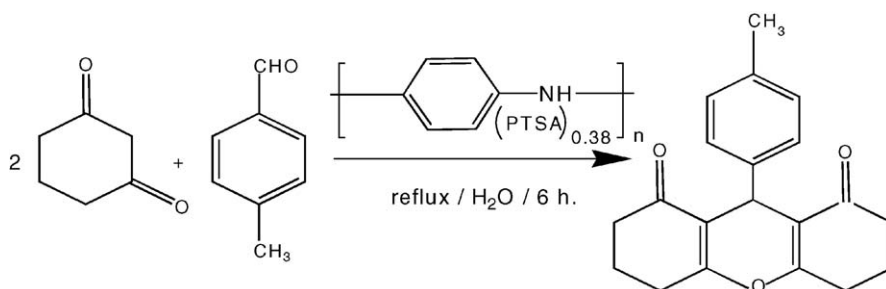
Beta zeolite supported on a  $\beta$ -SiC foam monolith: A diffusionless catalyst for fixed-bed Friedel–Crafts reactions


**Amalraj John, Palamari Jaya Prakash Yadav,  
Srinivasan Palaniappan**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 121

Clean synthesis of 1,8-dioxo-dodecahydroanthene derivatives catalyzed by polyaniline-*p*-toluenesulfonate salt in aqueous media

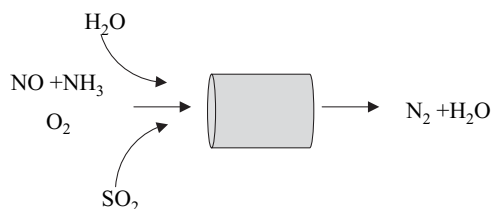
An efficient and straightforward procedure for the synthesis of 1,8-dioxo-dodecahydroanthene was achieved through one-pot condensation of arylaldehyde and 1,3-cyclohexanedione in the presence of polyaniline-*p*-toluenesulfonate salt as polymeric solid acid catalyst.


**Ramón Moreno-Tost, Enrique Rodríguez  
Castellón, Antonio Jiménez-López**

*Journal of Molecular Catalysis A: Chemical* 247 (2006) 126

Cobalt–iridium impregnated zirconium-doped mesoporous silica as catalysts for the selective catalytic reduction of NO with ammonia

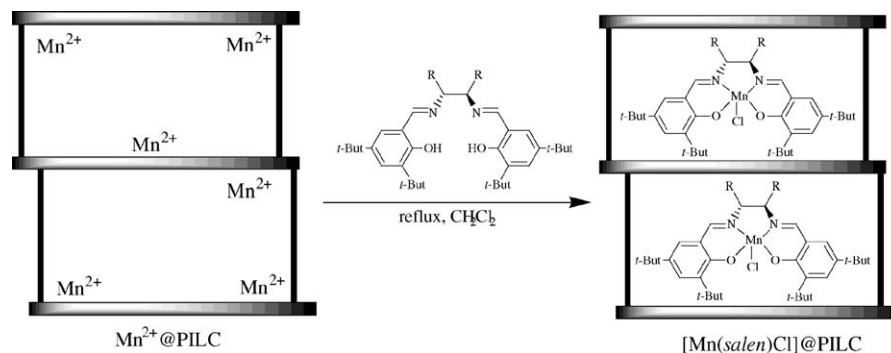
Cobalt–iridium tested in the selective catalytic reduction of NO with ammonia in an excess of oxygen are very active showing high conversions of NO. These catalysts maintain their activities when water is added to the feed on stream, but are less active with the addition of 100 ppm of SO<sub>2</sub>.



**Pankaj Das, Iwona Kuźniarska-Biernacka,  
Ana R. Silva, Ana P. Carvalho, João Pires,  
Cristina Freire**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 135

Encapsulation of chiral Mn(III) *salen* complexes into aluminium pillared clays: Application as heterogeneous catalysts in the epoxidation of styrene

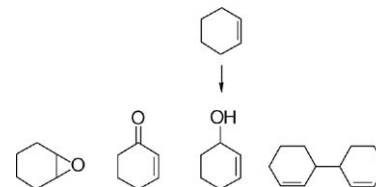


**Magdalena Zaręba, Marek Legięć,  
Bożena Sanecka, Jarosław Sobczak,  
Marek Hojniak, Stanisław Wołowicz**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 144

Catalytic decomposition of dimethyldioxirane and cyclic acetone triperoxide in presence of polynuclear complexes of cobalt(II,III) and copper(II)

Dimethyldioxirane and cyclic acetone triperoxide decompose in presence of polynuclear complexes of copper(II) and cobalt(II,III). The oxygen from these oxidants was found in products of oxidation of cyclohexene. The complexes trigger also the radical pathway of decomposition of dimethyldioxirane with hydroxyl, methyl and acetomethyl radicals involved.

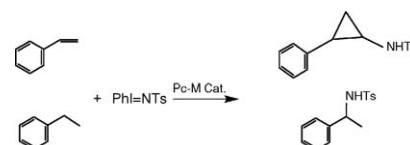


**Sheng-Yong Yan, Yi Wang, Yuan-Jie Shu,  
Hui-Hua Liu, Xiang-Ge Zhou**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 148

Nitrene transfer reaction catalyzed by substituted metallophthalocyanines

Metallophthalocyanines bearing substituents are found to be efficient catalysts for nitrene transfer reaction. Under optimized reaction conditions, aziridination of alkenes and amidation of C–H bonds with  $\text{PhI} = \text{NTs}$  by using 3-trifluoromethylphenoxy-substituted iron-phthalocyanine complex led to the highest yields of 90% and 85% for 4-methylstyrene and 4-methylethylbenzene, respectively.

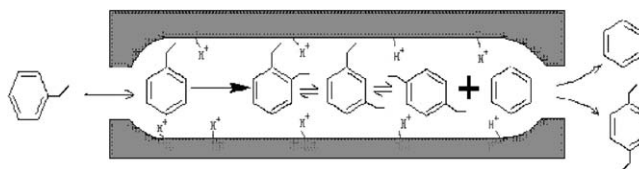


**Zhirong Zhu, Qingling Chen, Zaiku Xie,  
Weimin Yang, Dejin Kong, Can Li**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 152

Shape-selective disproportionation of ethylbenzene to *para*-diethylbenzene over ZSM-5 modified by chemical liquid deposition and MgO

The modified ZSM-5, for catalyzing shape-selective disproportionation of ethylbenzene to *para*-diethylbenzene, is prepared by chemical liquid deposition and loading MgO, which shows 98.6% high *para*-diethylbenzene selectivity and 28.1% ethylbenzene conversion with the low reactivity of dealkylation.

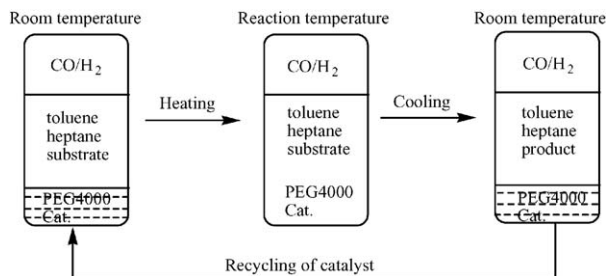


**Cuilan Feng, Yanhua Wang, Jingyang Jiang, Yuchuan Yang, Fengli Yu, Zilin Jin**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 159

Using thermoregulated PEG biphasic system to effect the hydroformylation of *p*-isobutylstyrene catalyzed by Rh/OPGPP complex

Thermoregulated PEG biphasic system, which is composed of PEG 4000 and mixture of toluene and heptane, was developed and used in the hydroformylation of *p*-isobutylstyrene (IBS) catalyzed by Rh/OPGPP complex. Under the optimum conditions, the conversion of IBS and yield of aldehyde are 99% and 96%, respectively. In addition, the catalyst could be easily separated from products and efficiently recovered.

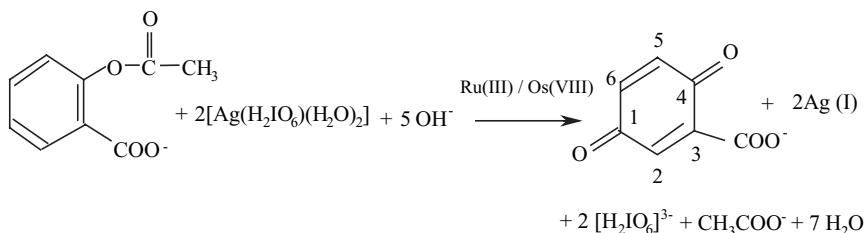


**Chanabasayya V. Hiremath, T.S. Kiran, Sharanappa T. Nandibewoor**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 163

Os(VIII)/Ru(III) catalyzed oxidation of aspirin drug by a new oxidant, diperioatoargentate(III) in aqueous alkaline medium: A comparative kinetic study

The oxidation reaction in alkaline medium has been shown to proceed via a Os(VIII)/Ru(III)–aspirin complex, which further reacts with one molecule of DPA in a rate determining step followed by other fast steps to give the products. The main products were identified by spot test, IR, NMR and GC–MS.

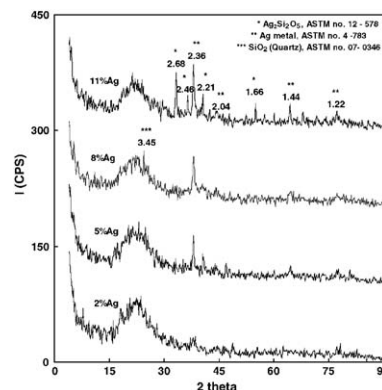


**Maged Samir Ghattas**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 175

Sodium-hypophosphite as a novel reducing agent in the preparation and characterization of silver/silica gel catalysts

New catalysts with different loading 2, 5, 8 and 11 wt.% silver on silica gel were prepared by chemical reduction method using a sodium-hypophosphite as a novel reducing agent. The structural changes were detected by XRD, DSC and IR techniques. Results show that ethanol dehydrogenation (at 300–450°C) was mainly dependent on the silver content and metal-support interaction. Catalyst sample containing 8% Ag was found the most active and selective for acetaldehyde formation and that contain 11% Ag is rich with silver silicate in certain mode. A texture property of the prepared catalysts was investigated.

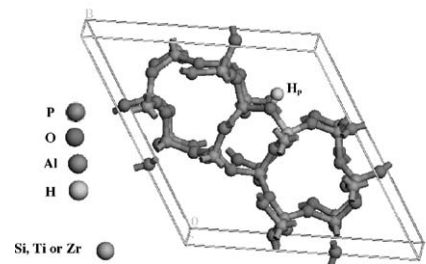


**M. Elanany, D.P. Vercauteren, M. Kubo, A. Miyamoto**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 181

The acidic properties of H-MeAlPO-5 (Me = Si, Ti, or Zr): A periodic density functional study

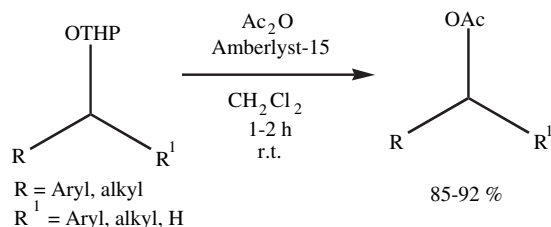
Density functional theory calculations on periodic models of aluminophosphate molecular sieves shows the relative acidity order: H-SiAlPO-5 > H-TiAlPO-5 > H-ZrAlPO-5. Furthermore, the Brønsted acidity of H-MeAlPO-5 (Me = Si or Ti) is weaker than those of their H-MeAlPO-34 counterparts.



**Biswanath Das, Majjigapu Ravinder Reddy,  
Kongara Ravinder, Reddy, Ravirala Ramu,  
Ponnaboina Thirupathi**

*Journal of Molecular Catalysis A: Chemical* 248  
(2006) 185

An efficient direct conversion of THP ethers into acetates using Amberlyst-15

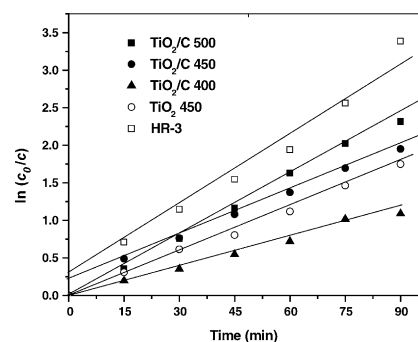


**Liuxue Zhang, Peng Liu, Zhixing Su**

*Journal of Molecular Catalysis A: Chemical* 248  
(2006) 189

A new route for preparation of TiO<sub>2</sub>/C hybrids and their photocatalytic properties

Linear transform  $\ln(C_0/C) = f(t)$  of the kinetic curves of MB depigmentation for different photocatalysts at 90 min of irradiation.

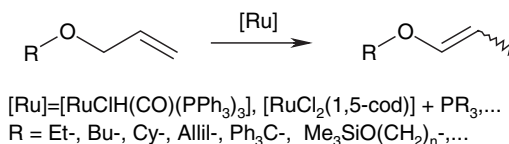


**Stanisław Krompiec, Nikodem Kuźnik,  
Magdalena Urbala, Józef Rzepa**

*Journal of Molecular Catalysis A: Chemical* 248  
(2006) 198

Isomerization of alkyl allyl and allyl silyl ethers catalyzed by ruthenium complexes

Double-bond migration in alkyl allyl and allyl silyl ethers was catalysed by ruthenium complexes. Mechanism of the reaction and catalyst recycling have been studied.

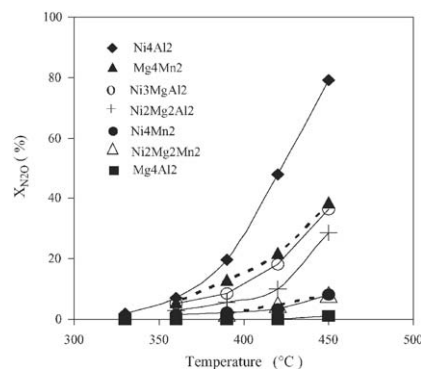


**L. Obalová, K. Jirátová, F. Kovanda,  
M. Valášková, J. Balabánová, K. Pacultová**

*Journal of Molecular Catalysis A: Chemical* 248  
(2006) 210

Structure-activity relationship in the N<sub>2</sub>O decomposition over Ni-(Mg)-Al and Ni-(Mg)-Mn mixed oxides prepared from hydrotalcite-like precursors

The decomposition of the nitrous oxide over catalysts prepared by thermal decomposition of Ni-(Mg)-M<sup>III</sup> (M<sup>III</sup> = Al or Mn) hydrotalcite-like precursors was studied. The Ni-Al and Mg-Mn catalysts exhibited high catalytic activity but those containing both transition metal cations (i.e. Ni and Mn) were less active. The activities of catalysts are connected with both the oxidation states of Ni and Mn and the amount of reducible components in the temperature range when the N<sub>2</sub>O decomposition proceeds. Up to a certain value of oxygen pressure, the presence of oxygen in the reaction mixture caused an inhibition of the reaction rate, while at higher oxygen pressures the N<sub>2</sub>O conversion remained nearly constant.



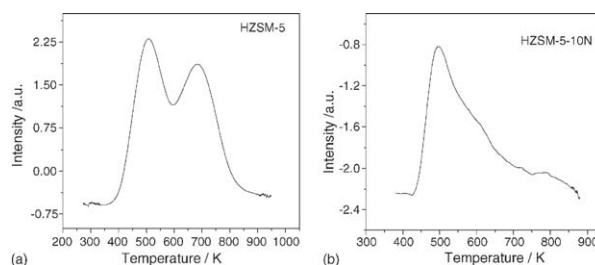


**Xinxin Guan, Na Li, Guangjun Wu, Jixin Chen, Fuxiang Zhang, Naijia Guan**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 220

Para-selectivity of modified HZSM-5 zeolites by nitridation for ethylation of ethylbenzene with ethanol

Patterns of  $\text{NH}_3$ -TPD for HZSM-5 and modified HZSM-5 zeolite with nitridation illustrated in Fig. 3 show that strong acid sites on modified HZSM-5 zeolite decreased severely, which indicated nitridation was mainly occurred on strong acid sites. The lost of strong acid sites provides high para-selectivity for ethylbenzene ethylation with ethanol.

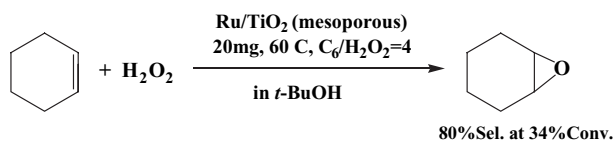


**Thammanoon Sreethawong, Yusuke Yamada, Tetsuhiko Kobayashi, Susumu Yoshikawa**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 226

Optimization of reaction conditions for cyclohexene epoxidation with  $\text{H}_2\text{O}_2$  over nanocrystalline mesoporous  $\text{TiO}_2$  loaded with  $\text{RuO}_2$

Reaction condition of  $\text{RuO}_2$  loaded on nanocrystalline mesoporous  $\text{TiO}_2$  with narrow and monomodal pore size distribution was optimized in terms of reaction temperature, catalyst amount and  $\text{H}_2\text{O}_2$  concentration on cyclohexene epoxidation activity with  $\text{H}_2\text{O}_2$  in *tert*-BuOH.

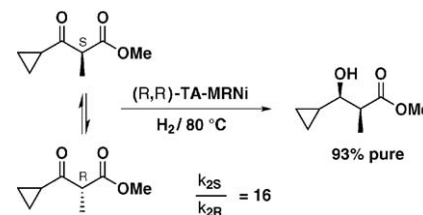


**Takashi Sugimura, Junya Watanabe, Satoshi Nakagawa, Tadashi Okuyama**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 233

Enantiomer-differentiating hydrogenation of methyl 3-cyclopropyl-2-methyl-3-oxopropanoate over tartaric acid-modified nickel. Performance of heterogeneous catalyst in dynamic kinetic resolution

A racemic mixture of methyl 3-cyclopropyl-2-methyl-3-oxopropanoate was hydrogenated over the tartaric acid-modified Raney nickel. Discrimination of the 2-methyl group during the reaction was high enough to perform the enantiomer differentiation,  $(2S)/(2R) = 16$ , and to cause an efficient dynamic kinetic resolution that resulted in one stereoisomer up to 93% of all the four hydrogenation products.



**Henk Hagen, Winfried P. Kretschmer, Frederik R. van Buren, Bart Hessen, Dominicus A. van Oeffelen**

*Journal of Molecular Catalysis A: Chemical* 248 (2006) 237

Selective ethylene trimerization: A study into the mechanism and the reduction of PE formation

The influence of catalyst activation on productivity and 1-hexene versus PE selectivity of titanium-based trimerization catalysts was studied. It was found that both could be improved largely by preactivation of the  $\text{Cp}^*\text{TiCl}_3$  catalyst in the absence of ethylene. The best results were achieved by using  $\text{Cp}^*\text{TiMe}_3$  catalysts.

