

## Contents

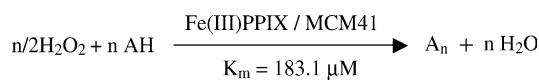
### Articles

**K. Nazari, S. Shokrollahzadeh, A. Mahmoudi, F. Mesbahi, N. Seyed Matin, A.A. Moosavi-Movahedi**

*Journal of Molecular Catalysis A: Chemical 239 (2005) 1*

Iron(III)protoporphyrin/MCM41 catalyst as a peroxidase enzyme model: Preparation and typical test reactions

MCM41 was synthesized and Fe(III)protoporphyrin(IX) (Fe(III)PPIX) was directly encapsulated into MCM41 pores through the self-assembly formation mechanism. Fe(III)PPIX/MCM41 was used in some typical and industrially important reactions. Kinetic parameters including rate constants, turnover number, Michaelis constant and catalytic efficiency were obtained. Results showed that Fe(III)PPIX/MCM41 catalyst is able to mimic horseradish peroxidase.

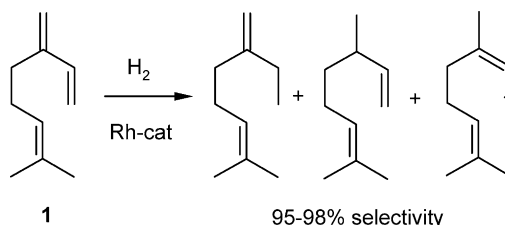


**Marcelo G. Speziali, Flávia C.C. Moura, Patricia A. Robles-Dutenhefner, Maria H. Araujo, Elena V. Gusevskaya, Eduardo N. dos Santos**

*Journal of Molecular Catalysis A: Chemical 239 (2005) 10*

Selective hydrogenation of myrcene catalyzed by complexes of ruthenium, chromium, iridium and rhodium

The hydrogenation of myrcene (1) catalyzed by Ru, Cr, Ir and Rh complexes leads to the formation of a complex mixture of mono-, di- and trihydrogenated products. Monohydrogenated products have been obtained with excellent combined selectivity of 95–98% at a high conversion of myrcene (>80%) by the appropriate choice of the catalyst and reaction conditions.

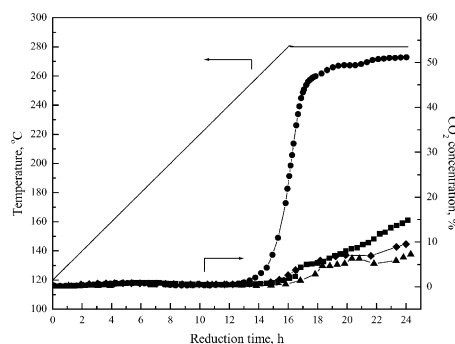


**Chenghua Zhang, Botao Teng, Yong Yang, Zhichao Tao, Qinglan Hao, Haijun Wan, Fan Yi, Binfu Xu, Hongwei Xiang, Yongwang Li**

*Journal of Molecular Catalysis A: Chemical 239 (2005) 15*

Effect of air-exposure on reduction behavior of a Fe–Mn–Cu–K/SiO<sub>2</sub> Fischer-Tropsch synthesis catalyst

Air-exposure suppresses the reduction behavior of Cu-promoted catalyst in Fischer-Tropsch synthesis, whereas, it does not affect that of Cu-free catalyst. The intrinsic reason of this phenomenon was investigated.

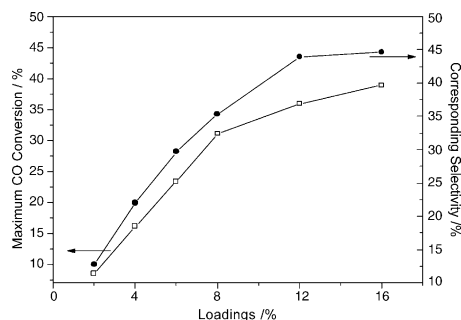


**Zhenping Qu, Mojie Cheng, Chuan Shi, Xinhe Bao**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 22

Low-temperature selective oxidation of CO in H<sub>2</sub>-rich gases over Ag/SiO<sub>2</sub> catalysts

Both the maximum CO conversion and the corresponding selectivity increase with the Ag loading, and the silver catalyst with higher loading may apply more active oxygen species for CO oxidation.

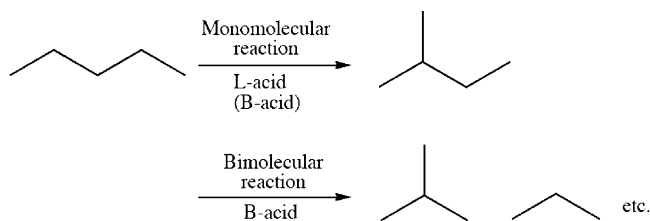


**Takemi Wakayama, Hiromi Matsuhashi**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 32

Reaction of linear, branched, and cyclic alkanes catalyzed by Brønsted and Lewis acids on H-mordenite, H-beta, and sulfated zirconia

Multi-branched alkanes showed higher reactivity than linear, mono-branched and cyclic alkanes. The highly selective isomerizations are considered to be catalyzed by Lewis acid sites. The bimolecular reaction takes place on Brønsted acid sites. Cyclohexane was converted into methylcyclopentane on both Brønsted and Lewis acid sites with high selectivity.



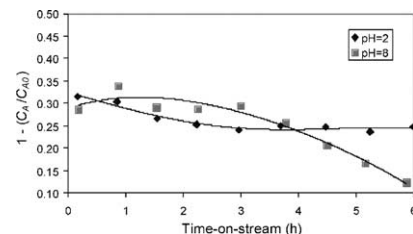
**Kelfin M. Hardiman, Cheng-Han Hsu, Tan T. Ying, Adesoji A. Adesina**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 41

The influence of impregnating pH on the postnatal and steam reforming characteristics of a Co-Ni/Al<sub>2</sub>O<sub>3</sub> catalyst

Bimetallic alumina supported Co-Ni catalysts were prepared by impregnation under low (2) and high (8) pH values. Higher dispersion and superior metal surface area at low-pH catalyst is ascribed to the charged-induced migration of metal cations towards the grain centre. On the other hand, in the high-pH catalyst, metal deposition occurred primarily around the pore mouth, and so blockage due to carbon lay-down would be more severe as the metal sites for hydrocarbon adsorption would be more readily accessible. However, as carbon build-up continues conversion appears to drop more quickly because of rapid loss of metal sites, whereas the more uniformly dispersed metal sites in pH 2 catalyst seems to maintain a steadier conversion level due to rela-

tively low carbon coverage. Post-mortem TOC analysis also confirmed that while pH 2 catalyst has a carbon content of 44%, pH 8 catalyst used under exactly the same S:C ratio possessed 56%.

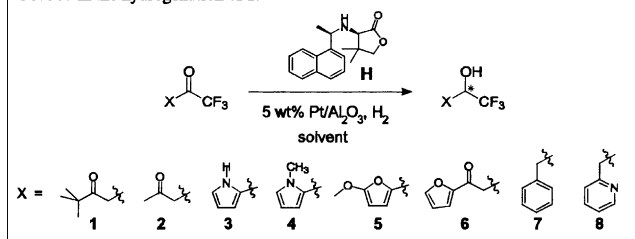


**Simon Diezi, Marco Hess, Elisabeth Orglmeister, Tamas Mallat, Alfons Baiker**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 49

Chemo and enantioselective hydrogenation of fluorinated ketones on platinum modified with (R)-1-(1-naphthyl)ethylamine derivatives

A series of chiral modifiers derived from (R)-1-(1-naphthylethyl)amine have been tested in the hydrogenation of fluorinated ketones (1-8) over Pt/Al<sub>2</sub>O<sub>3</sub>. Modifier H afforded 90% ee in the hydrogenation of 1.

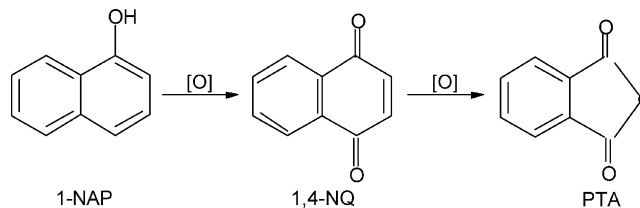


**S. Shylesh, S.P. Mirajkar, A.P. Singh**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 57

Influence of silica source in the catalytic activity and heterogeneity of mesoporous vanadosilicates

Mesoporous vanadosilicates were synthesized from two different silica sources, viz. fumed silica and tetraethyl orthosilicate, and were applied in the liquid phase oxidation reaction of 1-naphthol.

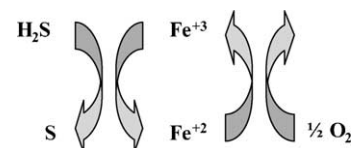


**Eun-Ku Lee, Kwang-Deog Jung, Oh-Shim Joo, Yong-Gun Shul**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 64

Influence of iron precursors on catalytic wet oxidation of H<sub>2</sub>S to sulfur over Fe/MgO catalysts

The Fe/MgO catalysts prepared from iron nitrate, iron chloride and iron sulfate were studied for catalytic wet oxidation of H<sub>2</sub>S to sulfur. Catalysts prepared from iron nitrate showed the highest H<sub>2</sub>S removal ability among the prepared catalysts. H<sub>2</sub>S removal ability correlates with the dispersion of iron oxide in the Fe/MgO catalysts.

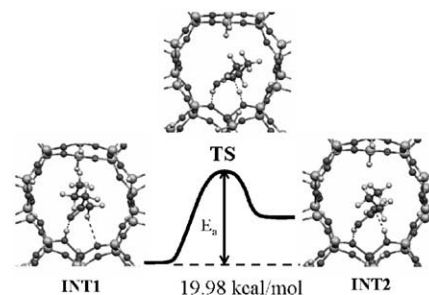


**Attasak Rattanasumrit, Vithaya Ruangpornvisuti**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 68

Theoretical study of conversion reactions of ketone to hydroxyalkylene in cluster models of zeolite H-ZSM-5

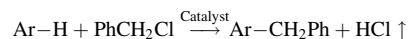
Conversions of acetaldehyde to hydroxyethylene, acetone to 2-hydroxypropylene, butanone to 2-hydroxybutene and 2-pentanone to 2-hydroxypentene catalyzed by H-ZSM-5 have been theoretically studied using quantum chemical methods. Three steps of the reaction mechanism were found and thermodynamic properties of each reaction steps and equilibrium constants of overall reaction have been obtained. The activation energies of all conversion reactions derived at three different methods are reported.



**Vasant R. Choudhary, Rani Jha, Vijay S. Narkhede**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 76

In-Mg-hydrotalcite anionic clay as catalyst or catalyst precursor for Friedel–Crafts type benzylation reactions



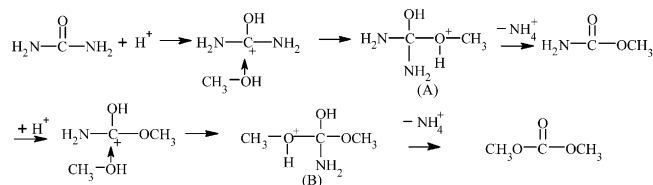
where Ar: benzene or substituted benzenes and catalyst: In-Mg-hydrotalcite anionic clay.

**Jianjun Sun, Bolun Yang, Xiaoping Wang, Dongpeng Wang, Hongye Lin**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 82

Synthesis of dimethyl carbonate from urea and methanol using polyphosphoric acid as catalyst

The synthesis of dimethyl carbonate from urea and methanol using polyphosphoric acid as catalyst has been studied and the following reaction mechanism has been proposed.

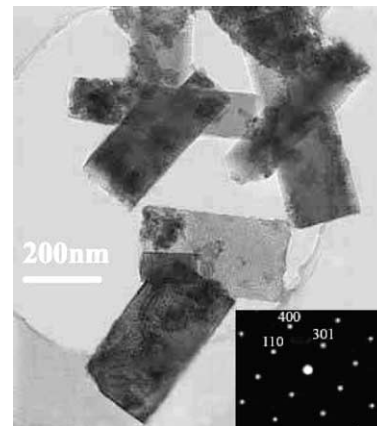


**ZhiQiang Song, HaiYan Xu, KunWei Li, Hao Wang, Hui Yan**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 87

Hydrothermal synthesis and photocatalytic properties of titanium acid  $\text{H}_2\text{Ti}_2\text{O}_5 \cdot \text{H}_2\text{O}$  nanosheets

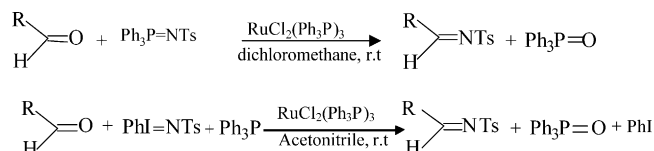
Titanium acid  $\text{H}_2\text{Ti}_2\text{O}_5 \cdot \text{H}_2\text{O}$  with nanosheet morphology has been prepared by doping  $\text{Zn}^{2+}$  into Ti-O crystal structure via a hydrothermal method. It demonstrated that  $\text{H}_2\text{Ti}_2\text{O}_5 \cdot \text{H}_2\text{O}$  show good photocatalytic properties in depigmentation of methyl orange solution by UV light irradiation.



**Suman L. Jain, Vishal B. Sharma, Bir Sain**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 92

Ruthenium catalyzed imido-transfer reactions of aldehydes: An easy access to *N*-sulfonyl aldimines under mild reaction conditions

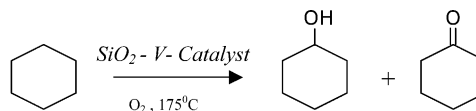


**Gopal S. Mishra, Armando J.L. Pombeiro**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 96

Selective single-pot oxidation of cyclohexane by molecular oxygen in presence of bis(maltolato) oxovanadium complexes covalently bonded to carbamated modified silica gel

Bis(maltolato)oxovanadium complexes have been covalently bonded to carbamated modified silica gel and shown to act as catalysts for the oxidation of cyclohexane by dioxygen, to cyclohexanol and cyclohexanone with a good activity and selectivity, without any additive and under relatively mild reactions. The effects of various factors were investigated towards the optimization of the reaction conditions and evidence is presented for a free-radical mechanism.

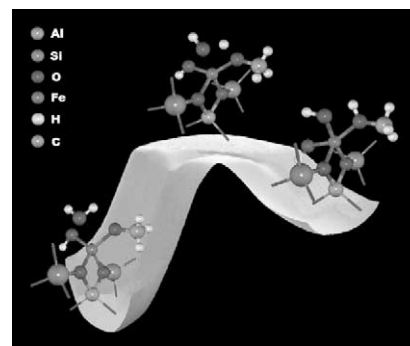


**Suwat Pabchanda, Piboon Pantu, Jumras Limtrakul**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 103

Hydrolysis of methoxide species and regeneration of active site in Fe-ZSM-5 catalyst by the ONIOM method

The methoxide species formed from methane oxidation on Fe-ZSM-5 catalyst can be readily hydrolyzed to form methanol. Then, the iron active site can be regenerated either by the direct dehydration or by the more energetically favorable pathway, water assisted condensation of hydroxyl groups following by desorption of water.

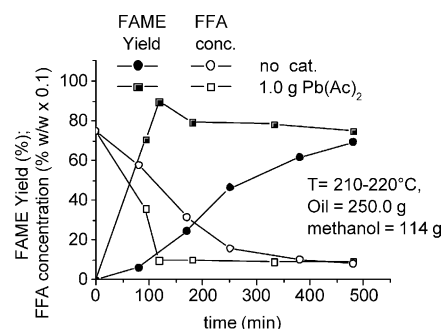


**M. Di Serio, R. Tesser, M. Dimiccoli, F. Cammarota, M. Nastasi, E. Santacesaria**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 111

Synthesis of biodiesel via homogeneous Lewis acid catalyst

The use of classical alkaline catalysts in the transesterification of waste fats and oils to obtain fatty methyl esters (FAME) poses great difficulties due to the presence of large amounts of free fatty acids (FFA). This paper studies as a possible alternative, the use of different bivalent metals. The most active catalysts have been individuated and a correlation of the activities with the cation acidity has been found.

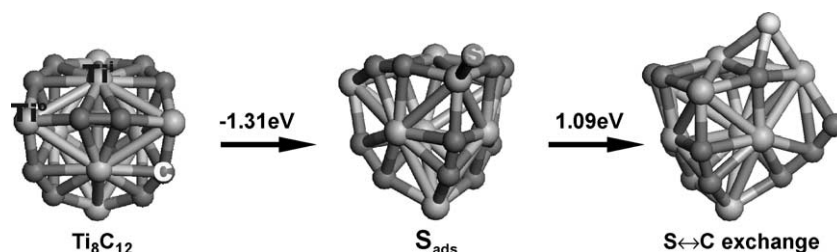


**Ping Liu, José A. Rodriguez, James T. Muckerman**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 116

Sulfur adsorption and sulfidation of transition metal carbides as hydrotreating catalysts

The adsorption of sulfur and sulfidation of transition metal carbides was investigated on extended surfaces  $MC(0\ 0\ 1)$  ( $M = \text{Ti, V, Mo, Ta}$ ),  $M_{14}C_{13}$  ( $M = \text{Ti, V, Mo}$ ) nanocrystals and  $M_8C_{12}$  ( $M = \text{Ti, V, Mo}$ ) metcar nanoparticles.  $M_8C_{12}$  metcars were found to be the best catalysts in this study for reactions involving sulfur and sulfur-containing molecules, being able to resist the sulfidation that leads to degradation of the carbides, while still bonding sulfur or breaking C-S bonds.

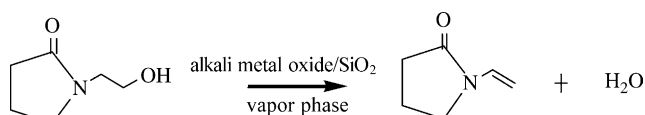


**Yuuji Shimasaki, Hitoshi Yano, Kimio Ariyoshi, Hideyuki Kambe**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 125

Vapor phase intramolecular dehydration of *N*-(2-hydroxyethyl)-2-pyrrolidone to *N*-vinyl-2-pyrrolidone over alkali metal oxide/SiO<sub>2</sub> catalysts

Newly developed alkali metal oxide/SiO<sub>2</sub> catalyst shows a high catalytic performance in the vapor phase intramolecular dehydration of *N*-(2-hydroxyethyl)-2-pyrrolidone to *N*-vinyl-2-pyrrolidone

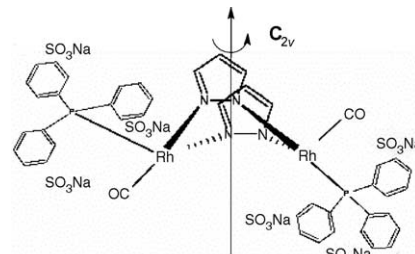


**P.J. Baricelli, Francisco López-Linares, A. Bruss, R. Santos, E. Lujano, R.A. Sánchez-Delgado**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 130

Biphasic hydroformylation of olefins by the new binuclear water soluble rhodium complex  $[\text{Rh}(\mu\text{-Pz})(\text{CO})(\text{TPPTS})_2]$

The synthesis and full characterization of the new water soluble complex  $[\text{Rh}(\mu\text{-Pz})(\text{CO})(\text{TPPTS})_2]$  is described. This complex was obtained by ligand exchange procedures and characterized by FT-IR,  $^1\text{H-NMR}$ ,  $^1\text{H}\{^31\text{P}\}\text{-NMR}$ , and  $^{31}\text{P-NMR}$ . These analyses confirmed that there are two pyrazolate bridging ligands in an exobidentate orientation, giving to the complex a  $\text{C}_{2v}$  symmetry. The complex was active in the catalytic hydroformylation of 1-hexene, styrene, allylbenzene, 2,3-dimethyl-1-butene, cyclohexene and their mixtures. Experiments shows that the binuclear complex is recyclable and resistant to possible sulphur poisons added to the reaction mixtures.

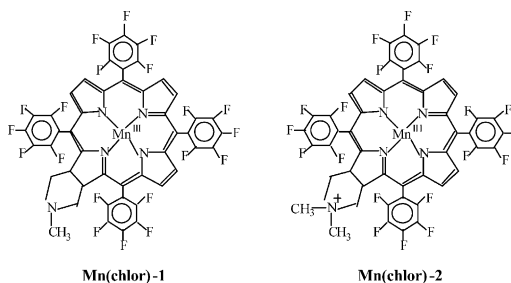


**Fábio S. Vinhado, Maria E.F. Gandini, Yassuko Iamamoto, Ana M.G. Silva, Mário M.Q. Simões, Maria G.P.M.S. Neves, Augusto C. Tomé, Susana L.H. Rebelo, Ana M.V.M. Pereira, José A.S. Cavaleiro**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 138

Novel Mn(III)chlorins as versatile catalysts for oxyfunctionalisation of hydrocarbons under homogeneous conditions

Novel Mn(III)chlorins have been obtained and used as efficient and versatile catalysts for oxyfunctionalisation of the cyclohexane with PhIO and  $\text{H}_2\text{O}_2$ . Mn(III)chlorin/ $\text{H}_2\text{O}_2$  should be oxidising the alkane by a concerted mechanism, whereas in Mn(III)chlorin/PhIO oxidations a free alkyl mechanism is operating, similarly to that observed in the oxidations catalysed by fluorinated Mn(II)porphyrins.

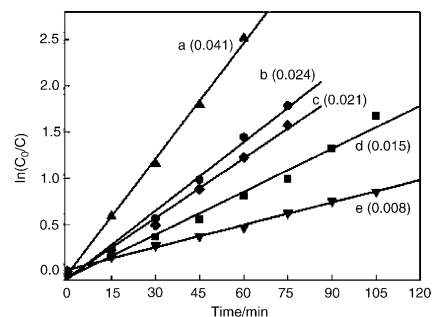


**Qiuqing Yang, Chao Xie, Zili Xu, Zhongmin Gao, Ziheng Li, Dejun Wang, Yaoguo Du**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 144

Effects of synthesis parameters on the physico-chemical and photoactivity properties of titania-silica mixed oxide prepared via basic hydrolyzation

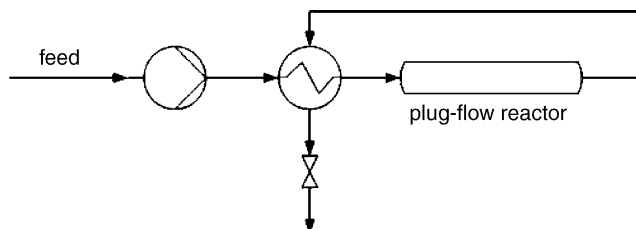
In this paper, we investigated the effects of a series of synthesis parameters, including synthesis route, aging time, the type of alcohol, and calcination temperature, on the physico-chemical and photoactivity of titania-silica mixed oxide prepared by using ammonia-water solution as the hydrolysis catalyst.



**M. Bicker, S. Endres, L. Ott, H. Vogel**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 151

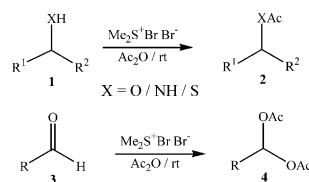
Catalytical conversion of carbohydrates in subcritical water: A new chemical process for lactic acid production



**Abu T. Khan, Samimul Islam, Adinath Majee, Tanmay Chattopadhyay, Subrata Ghosh**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 158

Bromodimethylsulfonium bromide: A useful reagent for acylation of alcohols, phenols, amines, thiols, thiophenols and 1,1-diacylation of aldehydes under solvent free conditions

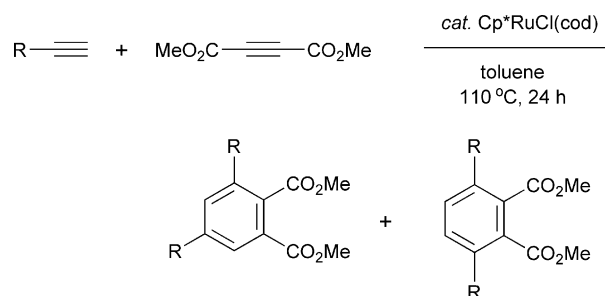


**Yasuyuki Ura, Yoshitaka Sato, Hiroshi Tsujita, Teruyuki Kondo, Misako Imachi, Take-aki Mitsudo**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 166

Ruthenium-catalyzed [2+2+2] cycloaddition of three different alkynes

A chemoselective [2+2+2] cycloaddition of an internal alkyne, a terminal alkyne and dimethyl acetylenedicarboxylate was efficiently catalyzed by Cp<sup>\*</sup>RuCl(cod) to give trisubstituted *o*-phthalates in good yield.

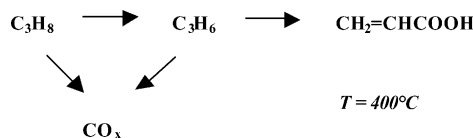


**G. Landi, L. Lisi, G. Russo**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 172

Oxidation of propane and propylene to acrylic acid over vanadyl pyrophosphate

Effects of operating parameters (temperature, contact time, water vapour and oxygen concentrations) were studied in propane mild oxidation of propane to acrylic acid (AA). Use of propylene as reactant was employed in order to better understand the reaction path. AA oxidation is inhibited up to 400°C leading to a quite purely parallel reaction scheme. Propane oxydehydrogenation appears the rate-limiting step.

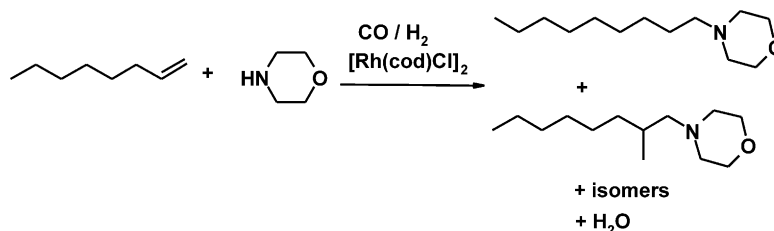


**Arno Behr, Reina Roll**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 180

Hydroaminomethylation in thermomorphic solvent systems

The use of temperature-dependent solvent systems (TMS systems) has been studied for the rhodium catalyzed hydroaminomethylation of 1-octene with morpholine. High conversions of the olefin up to 98% and high selectivities to the amines up to 96% can be obtained in TMS systems consisting of propylene carbonate, an alkane and a semi-polar mediator. After the reaction the catalyst can be easily recovered by a simple phase separation with only a negligible loss of the rhodium catalyst.

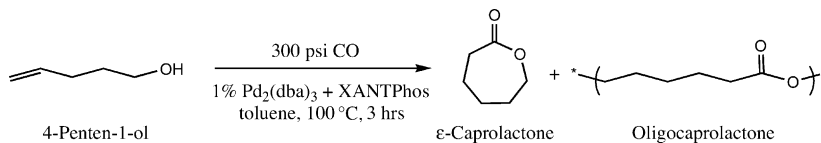


**Jeffrey K. Funk, David K. Newsham, David N. Goldstein, Shengsheng Liu, Ayusman Sen**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 185

Catalytic carbonylation of 4-penten-1-ol to  $\epsilon$ -caprolactone and oligocaprolactone

$\text{Pd}_2(\text{dba})_3 + \text{XANTPhos}$  in toluene is a catalyst for the alkoxycarbonylation of 4-penten-1-ol to  $\epsilon$ -caprolactone and 2-methylvalerolactone, as well as oligocaprolactone.

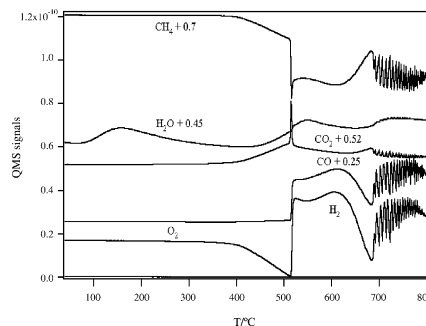


**Ying Liu, Wei Ping Fang, Wei Zheng Weng, Hui Lin Wan**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 193

Oscillations of partial oxidation of methane over H-ZSM-5 supported rhodium catalyst

The oscillatory behavior over the Rh/H-ZSM-5 catalyst was firstly reported at atmospheric pressure during the partial oxidation of methane, which may be attributed to the synergism of the formate species and the oxide with certain interaction with the support.

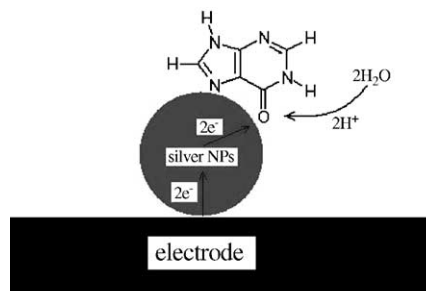


**Xiaoli Zhu, Xin Gan, Jing Wang, Ting Chen, Genxi Li**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 201

A new reduction route of hypoxanthine and its nonenzymatic detection based on silver nanoparticles

The interaction between hypoxanthine (HX) and silver nanoparticles (NPs) is studied with electrochemical technique, together with UV-vis spectroscopy (UV-vis) method. A new reduction route of HX corresponding to the transition from carbonyl to carboxyl at C6 of HX is found when HX adsorbs at silver NPs, and a nonenzymatic detection method for HX is constitute based on this new route.

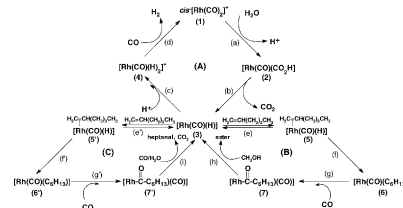


**Alvaro J. Pardey, Gabriela C. Uzcátegui, Fernando Hung-Low, Angel B. Rivas, Jorge E. Yáñez, Marisol C. Ortega, Clementina Longo, Pedro Aguirre, Sergio A. Moya**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 205

Hydroesterification versus hydroformylation-acetalization of 1-hexene catalyzed by soluble carbonylrhodium complexes of pyridine ligands

In this work, the hydroesterification and hydroformylation-acetalization of 1-hexene catalyzed by rhodium(I) complexes, *cis*-[Rh(CO)<sub>2</sub>(amine)<sub>2</sub>](PF<sub>6</sub>) (amine = pyridine, 2-picoline, 3-picoline, 4-picoline, 3,5-lutidine or 2,6-lutidine) dissolved in methanol under carbon monoxide atmosphere, is described. The reaction products distribution depends on the nature of the coordinated amine to the rhodium center. The effects of variation of CO pressure, temperature, catalyst concentration, 1-hexene/Rh molar ratio and reaction medium, on the reaction rates were also examined.

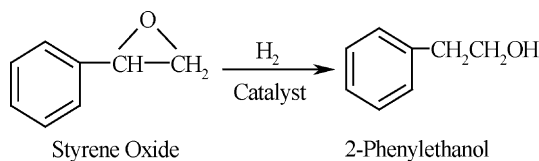




**I. Kirm, F. Medina, X. Rodríguez, Y. Cesteros, P. Salagre, J.E. Sueiras**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 215

Preparation of 2-phenylethanol by catalytic selective hydrogenation of styrene oxide using palladium catalysts

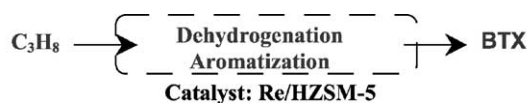


Gas-phase hydrogenation of styrene oxide to obtain 2-phenylethanol (2-PEA) using palladium catalysts on different supports was studied. The acid–base nature of the support played an important role in the selectivity. Acid support such as  $\text{Al}_2\text{O}_3$  or activated carbon favoured the formation of isomerization products, while a basic support such as  $\text{MgO}$  showed a high selectivity to 2-PEA.

**Jianjun Guo, Hui Lou, Hong Zhao, Lihe Zheng, Xiaoming Zheng**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 222

Dehydrogenation and aromatization of propane over rhenium-modified HZSM-5 catalyst



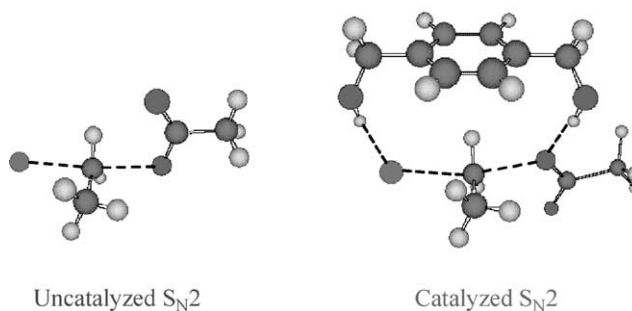
Re/HZSM-5 showed higher activity toward dehydrogenation and aromatization compared with HZSM-5 and Ga/HZSM-5 catalyst. Carbon dioxide largely inhibited the propane transformation, while methane improved the selectivity of aromatic products and inhibited the decomposition of propane.

**Josefredo R. Pliego Jr.**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 228

Design of an organocatalyst for ion–molecule  $\text{S}_{\text{N}}2$  reactions: A new solvent effect on the reaction rate predicted by ab initio calculations

Selective solvation of the  $\text{S}_{\text{N}}2$  transition state by the organocatalyst.

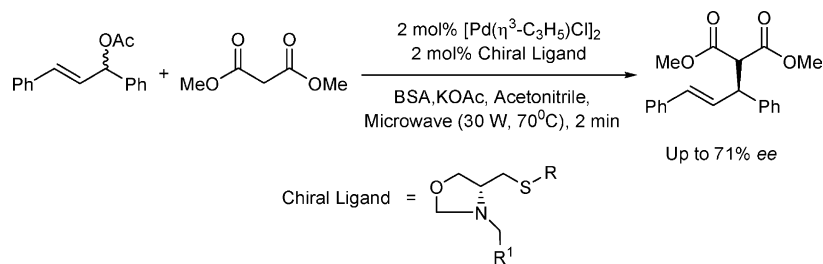


**Antonio L. Braga, Claudio C. Silveira, Martin W.G. de Bolster, Henri S. Schrekker, Ludger A. Wessjohann, Paulo H. Schneider**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 235

Microwave-accelerated asymmetric allylations using cysteine derived oxazolidine and thiazolidine palladium complexes

Microwave irradiation highly accelerates palladium-catalyzed enantioselective allylations with oxazolidine–thioether ligands and reduces the catalyst load required. However, sterically improved ligands giving high ee under normal conditions were not susceptible to such improvements.

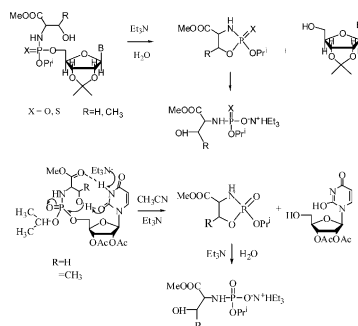


**Yuping Feng, Zhiwei Miao, Bo Han, Yufen Zhao**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 239

Kinetic and mechanistic studies on the dephosphoryl reaction catalyzed in nucleoside 5'-amino acid phosphoramidates

The dephosphoryl reactions catalyzed of nucleoside 5'-phosphoramidates, the kinetics and mechanisms of reaction are reported in this paper.

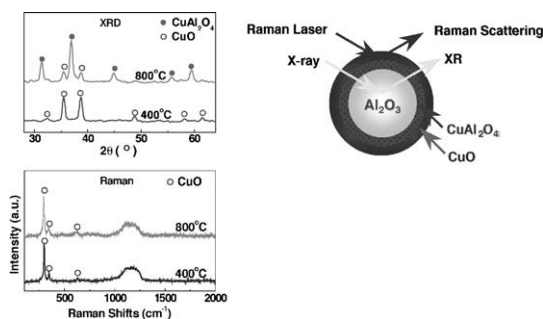


**Meng-Fei Luo, Ping Fang, Mai He, Yun-Long Xie**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 243

In situ XRD, Raman, and TPR studies of CuO/Al<sub>2</sub>O<sub>3</sub> catalysts for CO oxidation

Crystalline CuAl<sub>2</sub>O<sub>4</sub> has formed by solid–solid interaction between CuO and Al<sub>2</sub>O<sub>3</sub> at high temperatures. The formation of CuAl<sub>2</sub>O<sub>4</sub> inhibits CuO diffusing into Al<sub>2</sub>O<sub>3</sub> support. The CO oxidation activity is mainly related to the CuO species on the surface region of CuO/Al<sub>2</sub>O<sub>3</sub> catalysts.

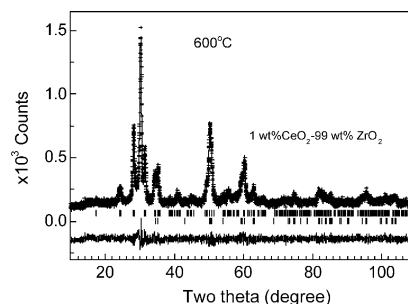


**J.A. Wang, T. López, X. Bokhimi, O. Novaro**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 249

Phase composition, reducibility and catalytic activity of Rh/zirconia and Rh/zirconia-ceria catalysts

Catalytic activity of the Rh loaded zirconia-ceria solid solution with cubic phase is quite higher than for the catalysts containing tetragonal and monoclinic phases of zirconia. The latter exhibited an inducing period in the reaction temperatures below 180°C on the catalytic activity profile that might be a result of the relatively low reducibility of these support.



**David Sémeril, Manuel Lejeune, Catherine Jeunesse, Dominique Matt**

*Journal of Molecular Catalysis A: Chemical* 239 (2005) 257

Heck, Suzuki and Kumada–Corriu cross-coupling reactions mediated by complexes based on the upper rim of diphosphinated calix[4]arenes

Two flexible bis-triarylphosphine chelators based on a calix[4]arene scaffold were assessed in combination with Pd or Ni as catalysts for C–C bond forming reactions involving aryl halides. Both ligands resulted in efficient catalysts for Heck, Suzuki and Kumada–Corriu cross-coupling reactions. The diphosphines were shown to be superior to PPh<sub>3</sub> when chlorobenzene was used as reagent.

