

## Contents

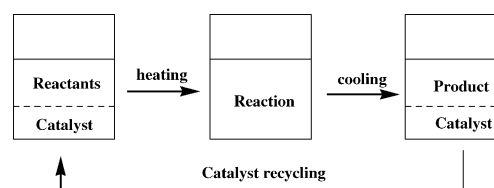
### Articles

Ya-dong Lu, Yan-hua Wang, Zi-lin Jin

*Journal of Molecular Catalysis A: Chemical 252 (2006) 1*

Thermoregulated *n*-heptane/poly(ethylene glycol) monoalkyl ether biphasic system and its application in PETPP/Ru complex catalyzed hydrogenation

A thermoregulated biphasic system composed of *n*-heptane and poly(ethylene glycol) (PEG) monoalkyl ether, which underwent a reversible change from biphasic to monophasic regulated by temperature, was reported and used for PETPP/Ru (PETPP = P-[*p*-C<sub>6</sub>H<sub>4</sub>O(CH<sub>2</sub>CH<sub>2</sub>O)<sub>*n*</sub>H]<sub>3</sub>, 3*n* = 14) complex catalyzed hydrogenation. After reaction, on cooling to room temperature, the catalyst-containing poly(ethylene glycol) monoalkyl ether phase could be easily separated from the product-containing *n*-heptane phase by simple decantation. The catalyst could be reused directly for the next run and the catalytic activity remained almost the same within ten successive runs.

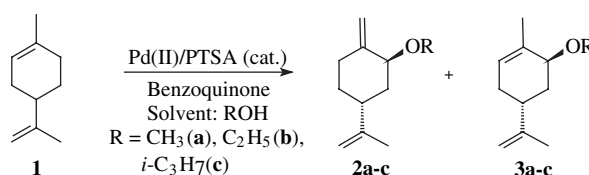


José Ailton Gonçalves, Aline C. Bueno, Elena V. Gusevskaya

*Journal of Molecular Catalysis A: Chemical 252 (2006) 5*

Palladium-catalyzed oxidation of monoterpenes: Highly selective syntheses of allylic ethers from limonene

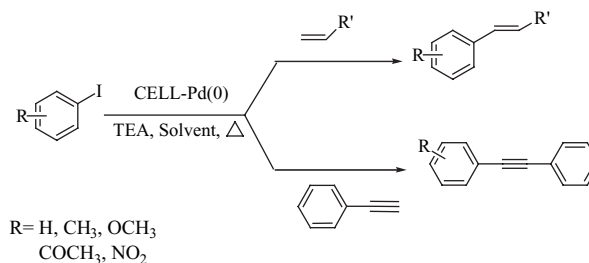
Selective syntheses of a series of allylic ethers **2a–c** and **3a–c**, which are potentially useful as fragrance ingredients, by the oxidation of limonene (**1**) with benzoquinone employing a Pd(II)/*p*-toluenesulfonic acid (PTSA) catalytic system were developed. A good control of regioselectivity was achieved through the appropriate choice of the ligand on palladium and reaction conditions.



K. Rajender Reddy, Nadakudity S. Kumar, P. Surendra Reddy, B. Sreedhar, M. Lakshmi Kantam

*Journal of Molecular Catalysis A: Chemical 252 (2006) 12*

Cellulose supported palladium(0) catalyst for Heck and Sonogashira coupling reactions



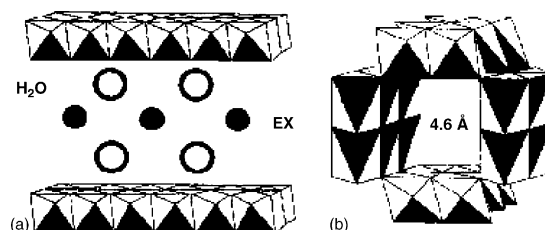


**R. Jothiramalingam, B. Viswanathan,  
T.K. Varadarajan**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 49

Synthesis, characterization and catalytic oxidation activity of zirconium doped K-OMS-2 type manganese oxide materials

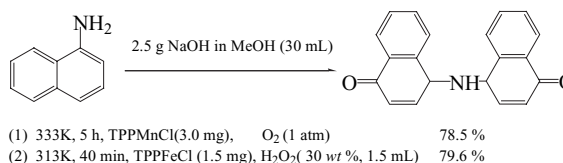
Zirconium doped manganese oxide OMS-2 materials have been synthesized. The synthesized zirconium doped manganese oxide OMS-2 materials have been characterized by XRD, TGA, BET and TEM techniques. Transmission electron micrographs showed the rod like needle shaped morphology and zirconia dispersion on fibrous morphology of as-synthesized zirconium doped manganese oxide OMS-2 materials. As synthesized zirconium incorporated OMS-2 catalysts have been tested for the liquid phase oxidation of side chain aromatic compounds (ethylbenzene and benzyl alcohol) and cyclohexanol.



**Tie Chen, Enhua Kang, Guiping Tan, Sijie Liu,  
Shaodan Zheng, Keer Yang, Shanling Tong,  
Chiguang Fang, Fengshou Xiao, Yan Yan**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 56

Highly selective catalytic preparation of bis(4-oxo-benzo-2-cyclohexen-1-yl) amine from 1-naphthylamine oxidation over metalloporphyrin catalysts by molecular oxygen under air pressure and by hydrogen peroxide.

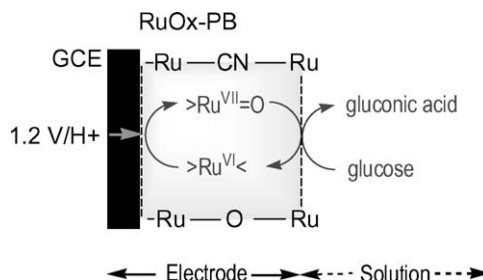


**Annamalai Senthil Kumar, Jyh-Myng Zen**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 63

Characteristic and electrocatalytic behavior of ruthenium Prussian blue analogue film in strongly acidic media.

Conceptual representation for the glucose oxidation at the electrogenerated  $>Ru^{VII}=O$  intermediate at the RuOx-PB in strongly acidic media.

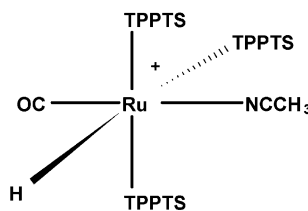


**P.J. Baricelli, K. Segovia, E. Lujano,  
M. Modroño-Alonso, Francisco López-Linares,  
R.A. Sánchez-Delgado**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 70

Synthesis and characterization of  $[HRu(CO)(CH_3CN)(TPPTS)_3]BF_4$ . Catalytic properties in the aqueous-biphasic hydroformylation of olefins.

The synthesis and characterization of the water soluble complex  $[HRu(CO)(CH_3CN)(TPPTS)_3]BF_4$  is described. This complex was obtained by ligand exchange procedures and characterized by FT-IR <sup>1</sup>H NMR, <sup>1</sup>H {<sup>31</sup>P} NMR and <sup>31</sup>P NMR techniques. These analyses confirmed that the ruthenium complex has a hexacoordinated arrangement. The complex was used as a catalytic precursor for the aqueous biphasic hydroformylation of several olefins and olefins mixtures. The observed catalytic activity was 1-hexane > allylbenzene > 2,3-dimethyl-1-butene > styrene > cyclohexene. The catalyst was shown to be resistant to sulphur positions.

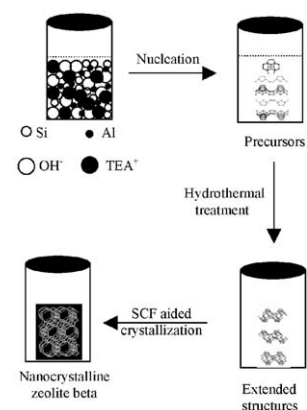


**M. Lakshmi Kantam, Bhavnari P.C. Rao, B.M. Choudary, K. Koteswara Rao, Bojja Sreedhar, Yasuhiro Iwasawa, Takehiko Sasaki**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 76

Synthesis of nanocrystalline zeolite beta in supercritical fluids, characterization and catalytic activity.

Nanocrystalline zeolite beta prepared in quantitative yields and in shorter crystallization times by applying a two-stage varying temperature synthesis and supercritical fluid aided crystallization has shown enhanced activity and selectivity towards 4-nitro-*o*-xylene in the nitration of *o*-xylene.

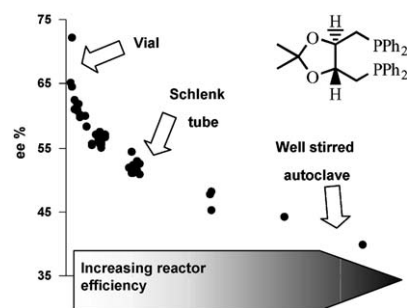


**Nathalie Pestre, Valérie Meille, Claude de Bellefon**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 85

Effect of gas-liquid mass transfer on enantioselectivity in asymmetric hydrogenations

The enantiomeric excess (ee) in asymmetric hydrogenation may vary with the concentration of dissolved hydrogen. Decrease of ee from 73 to less than 40% has been observed in the case of the Rh/diop catalysed hydrogenation of methyl-Z-( $\alpha$ )-acetamidocinnamate. The graphic sketches the importance of reactor type on the ee, which can lead to misleading interpretations on the structure-enantioselectivity relationship.

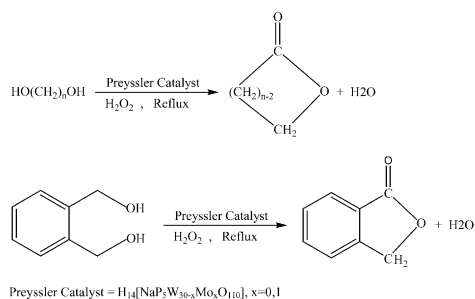


**Fatemeh F. Bamoharram, Majid M. Heravi, Mina Roshani, Ali Gharib, Manouchehr Jahangir**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 90

A catalytic method for synthesis of  $\gamma$ -butyrolactone,  $\epsilon$ -caprolactone and 2-cumaranone in the presence of Preyssler's anion,  $[\text{NaP}_5\text{W}_{30}\text{O}_{110}]^{14-}$ , as a green and reusable catalyst.

The catalytic lactonization of 1,4-butanediol, 1,6-hexanediol and 1,2-benzene dimethanol with Preyssler catalyst and hydrogen peroxide in various solvents was studied. The results show that in all cases molybdenum substituted Preyssler catalyst is the catalyst of choice. The effects of various parameters such as amount of diol, temperature, solvent and reaction time were studied.

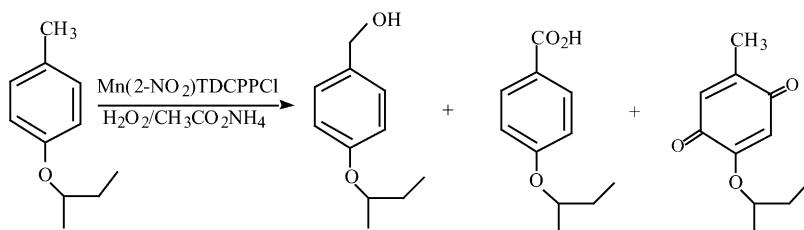


**Pietro Tagliatesta, Davide Giovannetti, Alessandro Leoni, Maria G.P.M.S. Neves, José A.S. Cavaleiro**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 96

Manganese(III) porphyrins as catalysts for the oxidation of aromatic substrates: An insight into the reaction mechanism and the role of the cocatalyst

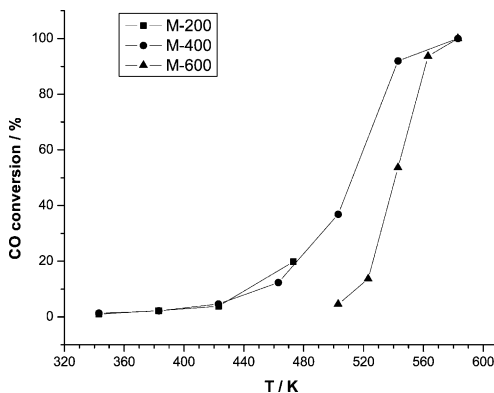
The oxidation of aromatic compounds by hydrogen peroxide catalysed by manganese porphyrins is inhibited by the final phenolic products. When the reaction is performed on the *sec*-butyl or *tert*-butyldimethylsilyl ethers of 4-methylphenol, the oxidation gives a mixture of the benzyl alcohol and benzoic acid derivatives in moderate yield. In the case of the *sec*-butyl ether a quinone derivative is also produced



**Goran Šmit, Stanka Zrnčević, Károly Lázár**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 103

Adsorption and low-temperature oxidation of CO over iron oxides

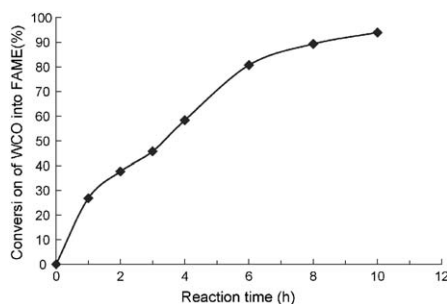


**Yong Wang, Shiyi Ou, Pengzhan Liu, Feng Xue, Shuze Tang**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 107

Comparison of two different processes to synthesize biodiesel by waste cooking oil.

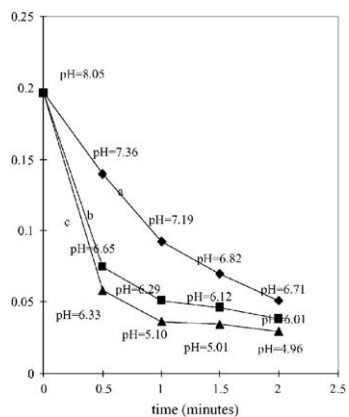
In this work, a comparative study on preparation of biodiesel by the waste cooking oil (WCO) by two different processes was conducted. One process was traditional acid catalyzed one, in which the synthesis of biodiesel was catalyzed by sulfur acid, but the other process was a new two-step catalyzed one.



**Yu Zhiyong, Liubov Kiwi-Minsker, Albert Renken, John Kiwi**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 113

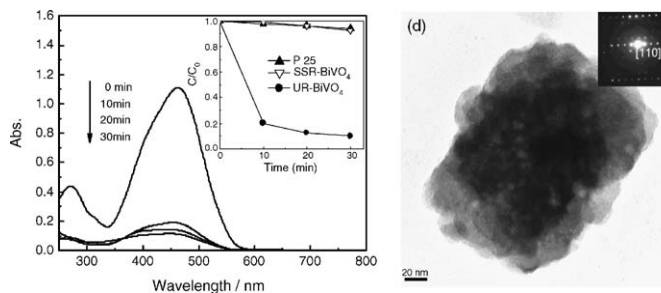
Detoxification of diluted azo-dyes at biocompatible pH with the oxone/Co<sup>2+</sup> reagent in dark and light processes



**Lin Zhou, Wenzhong Wang, Shengwei Liu, Lisha Zhang, Haolan Xu, Wei Zhu**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 120

A sonochemical route to visible-light-driven high-activity BiVO<sub>4</sub> photocatalyst

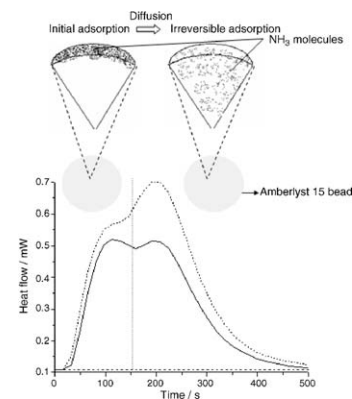


**Prem Felix Siril, David R. Brown**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 125

Acid site accessibility in sulfonated polystyrene acid catalysts: Calorimetric study of  $\text{NH}_3$  adsorption from flowing gas stream

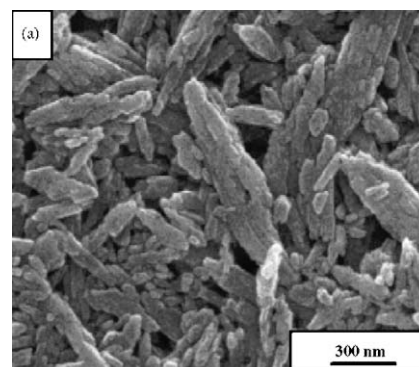
Calorimetric pulsed  $\text{NH}_3$  adsorption measurements from a flowing carrier gas have been made on sulfonated poly(styrene-*co*-divinylbenzene) resin acid catalysts to characterise surface acidity in general and acid site accessibility in particular. Results are interpreted in terms of an adsorption process as depicted below.

**Lin-Rui Hou, Chang-Zhou Yuan, Yang Peng**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 132

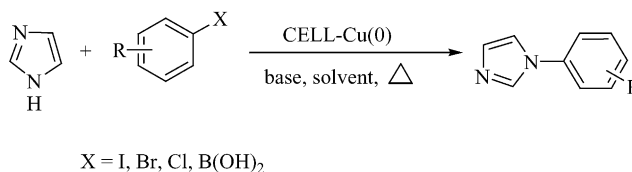
Preparation and photocatalytic property of sunlight-driven photocatalyst  $\text{Bi}_{38}\text{ZnO}_{58}$

Sunlight-driven photocatalyst  $\text{Bi}_{38}\text{ZnO}_{58}$  was synthesized by a solid-state reaction method. The product was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The photocatalytic degradation of methylene blue was evaluated, and the possible pathway of the photocatalytic reaction also has been studied. In addition, the band edge position of  $\text{Bi}_{38}\text{ZnO}_{58}$  was roughly calculated.

**K. Rajender Reddy, Nadakuditi S. Kumar, B. Sreedhar, M. Lakshmi Kantam**

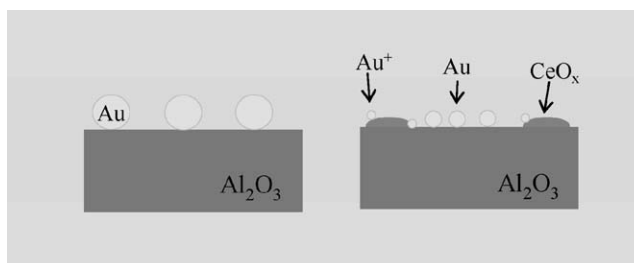
*Journal of Molecular Catalysis A: Chemical* 252 (2006) 136

*N*-Arylation of nitrogen heterocycles with aryl halides and arylboronic acids catalyzed by cellulose supported copper(0)

**M.A. Centeno, K. Hadjiivanov, Tz. Venkov, Hr. Klimev, J.A. Odriozola**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 142

Comparative study of  $\text{Au}/\text{Al}_2\text{O}_3$  and  $\text{Au}/\text{CeO}_2\text{-Al}_2\text{O}_3$  catalysts.

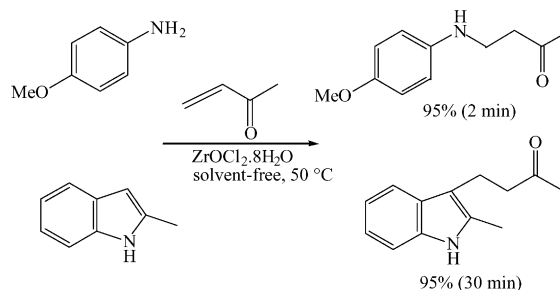


**Habib Firouzabadi, Nasser Iranpoor,  
Maasoumeh Jafarpour, Arash Ghaderi**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 150

ZrOCl<sub>2</sub>·8H<sub>2</sub>O as a highly efficient and the moisture tolerant Lewis acid catalyst for Michael addition of amines and indoles to α, β-unsaturated ketones under solvent-free conditions

ZrOCl<sub>2</sub>·8H<sub>2</sub>O as a safe, inexpensive, air and moisture tolerant Lewis acid catalyst were used for efficient Michael addition of indoles and amines to cyclic and acyclic α, β-unsaturated ketones under solvent-free conditions at 50 °C without any side reactions. The catalyst successfully reused several times for next round of reactions.

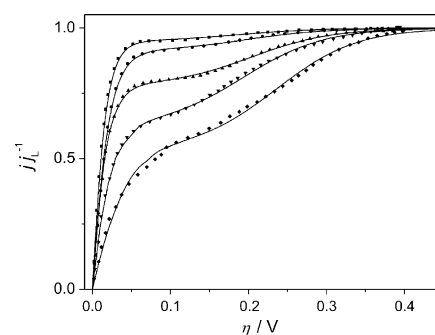


**P.M. Quaino, J.L. Fernández,  
M.R. Gennero de Chialvo, A.C. Chialvo**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 156

Hydrogen oxidation reaction on microelectrodes:  
Analysis of the contribution of the kinetic routes

The experimental behavior of the hydrogen oxidation reaction on platinum microelectrodes has been explained on the basis of a rigorous kinetic treatment involving the Tafel–Heyrovsky–Volmer mechanism. It has been found that such behavior is due to the significant variation of the reaction rates of the Tafel–Volmer and Heyrovsky–Volmer routes with overpotential.

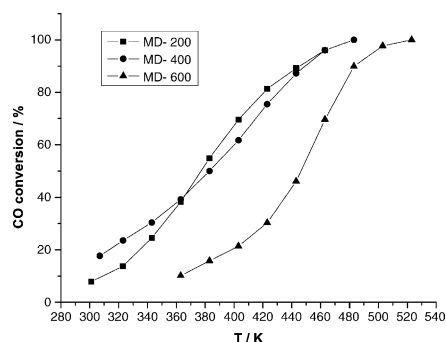


**Goran Šmit, Neven Strukan, Menno W.J. Crajé,  
Károly Lázár**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 163

A comparative study of CO adsorption and oxidation on Au/Fe<sub>2</sub>O<sub>3</sub> catalysts by FT-IR and in situ DRIFTS spectroscopies

Influences of different iron oxides, used as gold supports, on CO oxidation were tested by FT-IR spectroscopy during adsorption of CO in a vacuum and by DRIFTS spectroscopy in the reaction conditions. The investigation showed that the adsorption and oxidation are independent of chemical composition and structure of the supports, but that they depend only in presence of surface –OH groups. The catalyst without –OH groups had significantly less activity despite the fact that it is almost identical in chemical composition and structure to one of the active catalysts.

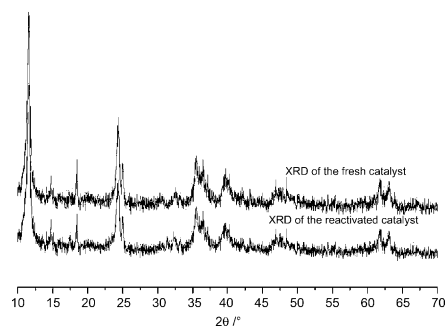


**Chun-Xia Chen, Cheng-Hua Xu,  
Liang-Rong Feng, Fa-Li Qiu, Ji-Shuan Suo**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 171

Deactivation and reactivation of copper-containing pentatomic hydrotalcite in catalytic hydroxylation of phenol

The phenol hydroxylation catalyzed over copper-containing pentatomic hydrotalcite (Cu-PHTL) is investigated during the catalyst cycle lifetime. The deactivated catalyst is easily reactivated, moreover, the reactivated catalyst shows almost the same catalytic performances and hydrotalcite structure as the fresh one.

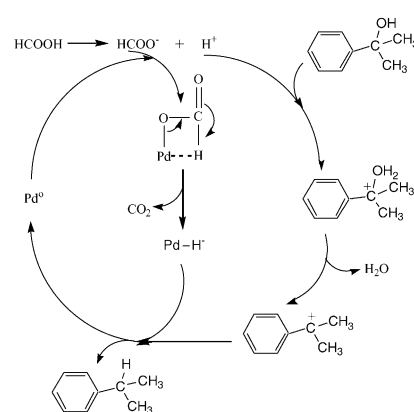


**Xiaohui Liu, Guanzhong Lu, Yanglong Guo, Yun Guo, Yunsong Wang, Xinhong Wang**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 176

Catalytic transfer hydrogenolysis of 2-phenyl-2-propanol over palladium supported on activated carbon

Catalytic transfer hydrogenolysis of 2-phenyl-2-propanol over Pd/C with formic acid

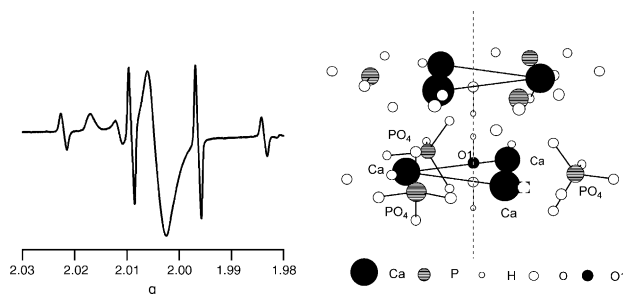


**Hiroyoshi Kanai, Masami Lintuluoto, Yasuyuki Matsumura, John B. Moffat**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 181

ESR study of the active oxygen species on hydroxyapatite activated by heat treatment

Hydroxyapatite was heated at 973 K followed by reacting with O<sub>2</sub> to give O<sub>2</sub><sup>-</sup>. The O<sub>2</sub><sup>-</sup> species rapidly reacted with propylene at room temperature. Then the hydroxyapatite was heated at 873K followed by treating with O<sub>2</sub> to give a quartet signal ( $g = 2.002$ ,  $a = 2.15$  mT) derived from the interaction between the newly formed unpaired electron and three equivalent phosphorus atoms.

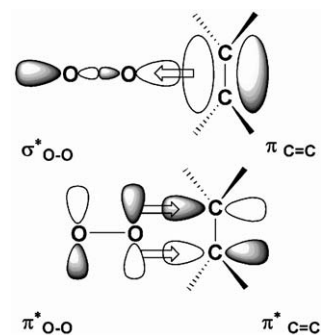


**Juliana M. de S. e Silva, Fábio S. Vinhado, Dalmo Mandelli, Ulf Schuchardt, Roberto Rinaldi**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 186

The chemical reactivity of some terpenes investigated by alumina catalyzed epoxidation with hydrogen peroxide and by DFT calculations

The selectivity of the alumina catalyzed epoxidation of (*S*)-limonene, citronelal, citral, citronelol and (1*S*)-( $\alpha$ )-pinene with aqueous 70 wt% and anhydrous 24 wt% hydrogen peroxide is described. DFT molecular orbital calculations were used for a better understanding of the reactivity of these terpenes. The more nucleophilic carbon-carbon double bond, which has a higher molecular orbital energy, is preferentially oxidized and a preference for the epoxidation in competition with other possible reactions is observed.

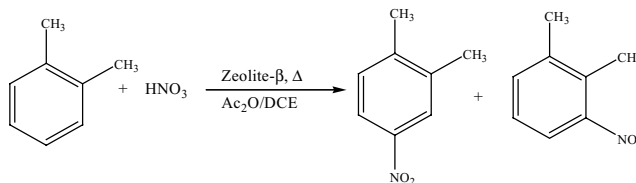


**V.N. Sheemol, B. Tyagi, R.V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 194

Nitration of *o*-xylene over rare earth cations exchanged zeolite- $\beta$  with nitric acid and acetic anhydride.

The catalytic activity of rare earth cations exchanged zeolite- $\beta$  was studied for the nitration of *ortho*-xylene with acetic anhydride and dichloroethane as solvents in liquid phase. Higher conversion observed with acetic anhydride solvent is explained in terms of acetyl nitrate formed as intermediate species.



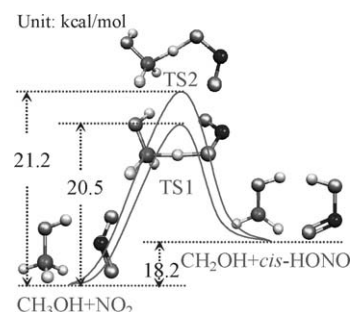


**Chao-Xian Xiao, Ning Yan, Ming Zou,  
Si-Cong Hou, Yuan Kou, Wenjian Liu,  
Shaowen Zhang**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 202

NO<sub>2</sub>-catalyzed deep oxidation of methanol:  
Experimental and theoretical studies

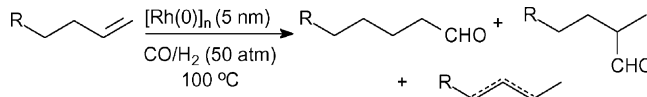
On-line infrared (IR) and in situ IR investigations show that a trace amount of NO<sub>x</sub> (for example, 600 ppm NO and/or NO<sub>2</sub>) can dramatically promote the oxidation of methanol. NO<sub>2</sub> was found to be the active catalyst during this process by both experiments and theoretical calculations. Two most favorite pathways were found, yielding CH<sub>2</sub>OH and *cis*-HONO as the products.



**Arnoldo J. Bruss, Marcos A. Gelesky,  
Giovanna Machado, Jairton Dupont**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 212

Rh(0) nanoparticles as catalyst precursors for the  
solventless hydroformylation of olefins.

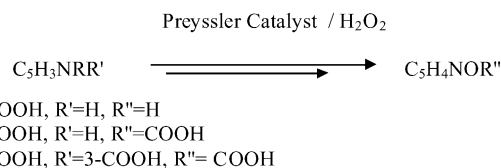


**Fatemeh F. Bamoharram, Majid M. Heravi,  
Mina Roshani, Niloofar Tavakoli**

*Journal of Molecular Catalysis A: Chemical* 252  
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N-oxidation of pyridine carboxylic acids using  
hydrogen peroxide catalyzed by a green heteropoly-  
acid catalyst: Preyssler's anion, [NaP<sub>5</sub>W<sub>30</sub>O<sub>110</sub>]<sup>14-</sup>

Preyssler heteropolyacid with exclusive properties and along with retention of structure, in the presence of hydrogen peroxide catalyzes N-oxidation of the pyridine carboxylic acids to the related N-oxides with decarboxylation in 2-position with respect to nitrogen.

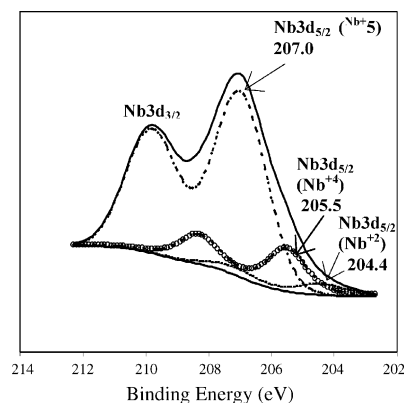


**Susana Martínez-Méndez, Yurgenis Henríquez,  
Olgioly Domínguez, Lindora D'Ornelas,  
Heinz Krentzien**

*Journal of Molecular Catalysis A: Chemical* 252  
(2006) 226

Catalytic properties of silica supported titanium,  
vanadium and niobium oxide nanoparticles towards  
the oxidation of saturated and unsaturated hydrocarbons

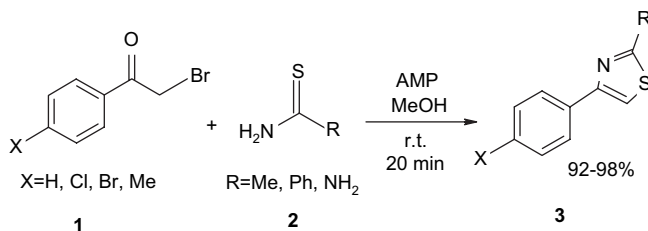
Silica supported nanostructured oxide systems of titanium (1.9 nm), vanadium (2.3 nm) and niobium (1.6 nm) were synthesized by reduction of the respective metallic chlorides. These materials were characterized by ICP-OES, FTIR, HRTEM and XPS analyses. The synthesized systems showed high activity and selectivity in the catalytic oxidation of 1-hexene, cyclohexene and cyclohexane in the presence of TBHP and oxygen as oxidizing agents.



**Biswanath Das, V. Saidi Reddy, R. Ramu**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 235

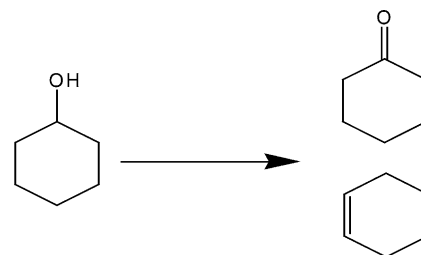
A rapid and high-yielding synthesis of thiazoles and aminothiazoles using ammonium-12-molybdophosphate.

**Benjaram M. Reddy, K. Jeeva Ratnam, Pranjali Saikia**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 238

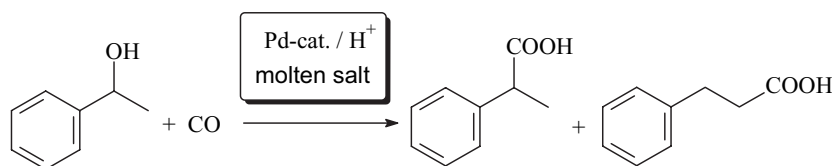
Characterization of CaO-TiO<sub>2</sub> and V<sub>2</sub>O<sub>5</sub>/CaO-TiO<sub>2</sub> catalysts and their activity for cyclohexanol conversion.

Influence of CaO on TiO<sub>2</sub>-anatase phase stabilization and dispersion of V<sub>2</sub>O<sub>5</sub> over CaO-TiO<sub>2</sub> have been investigated using different techniques. The CaO-TiO<sub>2</sub> and V<sub>2</sub>O<sub>5</sub>/CaO-TiO<sub>2</sub> exhibit more selectivity towards cyclohexanone and cyclohexene, respectively, reflecting their acid-base properties.

**Albert Lapidus, Oleg Eliseev, Tatyana Bondarenko, Nikolaj Stepin**

*Journal of Molecular Catalysis A: Chemical* 252 (2006) 245

Palladium catalysed hydroxycarbonylation of 1-phenylethanol in molten salt media

**Heesoo Kim, Min Hye Youn, Ji Chul Jung, In Kyu Song**

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UV-visible absorption edge energy of heteropolyacids (HPAs) as a probe of catalytic performance of HPAs in the oxidative dehydrogenation of isobutyric acid

The absorption edge energies of heteropolyacid (HPA) catalysts measured by UV-visible spectroscopy were correlated with the catalytic performance of HPA catalysts in the oxidative dehydrogenation of isobutyric acid. It was revealed that the absorption edge energies could be utilized as a correlation parameter for the reduction potentials (oxidizing powers) of the HPA catalysts, and furthermore, as a probe of catalytic oxidation performance of the HPA catalysts.

