

## Contents

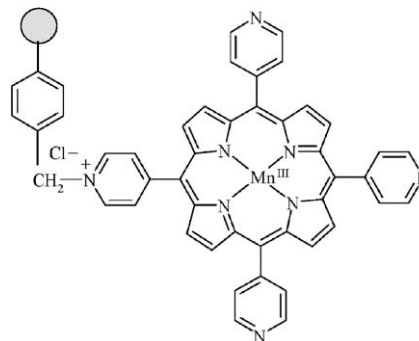
### Articles

**Majid Moghadam, Shahram Tangestaninejad, Mohammad Hosein Habibi, Valiollah Mirkhani**

*Journal of Molecular Catalysis A: Chemical 217 (2004) 9*

A convenient preparation of polymer-supported manganese porphyrin and its use as hydrocarbon monooxygenation catalyst

An easy method for preparing new cross-linked polystyrene-manganese(III) porphyrin resin is reported, which was found to be an efficient catalyst for alkene epoxidation and alkane hydroxylation by sodium periodate.

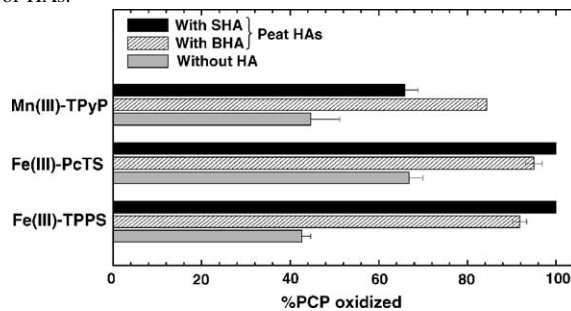


**Sinta Rismayani, Masami Fukushima, Akira Sawada, Hiroyasu Ichikawa, Kenji Tatsumi**

*Journal of Molecular Catalysis A: Chemical 217 (2004) 13*

Effects of peat humic acids on the catalytic oxidation of pentachlorophenol using metalloporphyrins and metallophthalocyanines

The catalytic oxidation of pentachlorophenol with Fe(III)- or Mn(III)-porphyrins and phthalocyanines was enhanced significantly by adding peat humic acids (HAs). This can be attributed to the interactions between catalysts and polysaccharide parts in HAs. Such interactions were observed by the visible absorption spectra of Fe(III)-porphyrin in the presence of HAs or hydroxypropyl- $\beta$ -cyclodextrin that was used as a model of HAs.

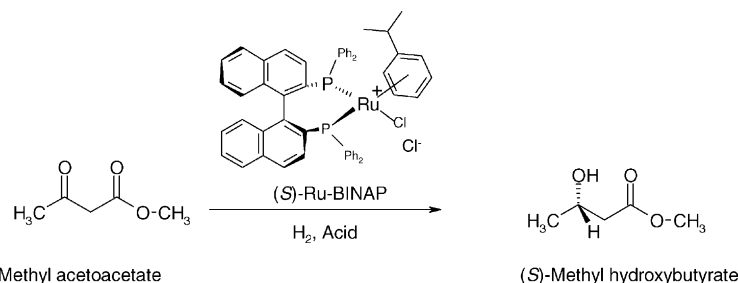


**Adi Wolfson, Ivo F.J. Vankelecom, Shimona Geresh, Pierre A. Jacobs**

*Journal of Molecular Catalysis A: Chemical 217 (2004) 21*

The role of acid in accelerating the asymmetric reduction of methyl acetoacetate with BINAP-chloro-(*p*-cymene)-Ru chloride complex

The effect of addition of organic and inorganic catalytic amounts of acid on the asymmetric hydrogenation of methyl acetoacetate with Ru-BINAP complex was studied.

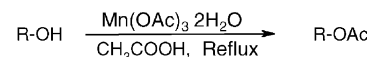


**Sidde Gowda, K.M. Lokanatha Rai**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 27

Manganese(III) acetate as catalyst for the direct acetylation of alcohols with acetic acid

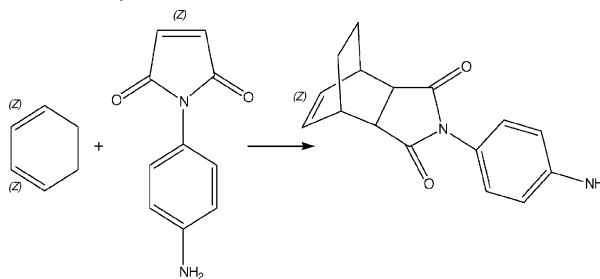
Manganese(III) acetate was found to catalyse the direct acetylation of primary, secondary and tertiary alcohols in presence of glacial acetic acid

**Elena Busi, Riccardo Basosi, Fabio Ponticelli, Massimo Olivucci**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 31

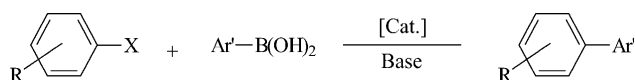
An innovative approach to the design of plastic antibodies: molecular imprinting via a non-polar transition state analogue

A plastic antibody, imprinted with a transition state analogue which possesses a dominant non-polar structure, was synthesized. This acrylic resin catalyzes the Diels–Alder reaction with an efficiency comparable to that of a recently developed monoclonal catalytic antibody. We argue that plastic antibodies can be successfully used to catalyze reactions with a transition state of low polarity. Moreover they represent a flexible catalyst when varied reaction conditions and solvent environments are needed.

**İsmail Özdemir, Bülent Alıcı, Nevin Gürbüz, Engin Çetinkaya, Bekir Çetinkaya**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 37

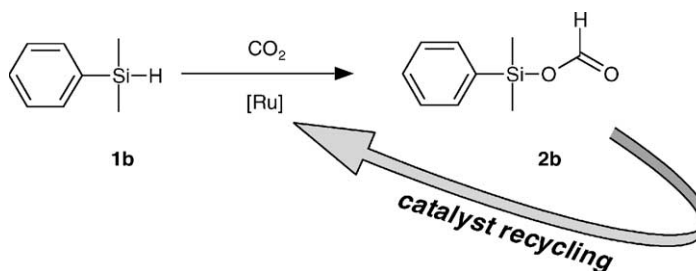
In situ generated palladium catalysts bearing 1,3-dialkylperimidin-2-ylidene ligands for Suzuki reactions of aryl chlorides

**Achim Jansen, Stephan Pitter**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 41

Homogeneously catalysed reduction of carbon dioxide with silanes: a study on solvent and ligand effects and catalyst recycling

Ruthenium catalysts exhibit excellent activities for the hydrosilylation of  $\text{CO}_2$ . The activity is enhanced with nitriles as solvent and by utilisation of phosphine ligands. Thermal separation of the reaction product makes possible an efficient catalyst recycling, as confirmed by 10 successive runs without loss of catalytic activity.



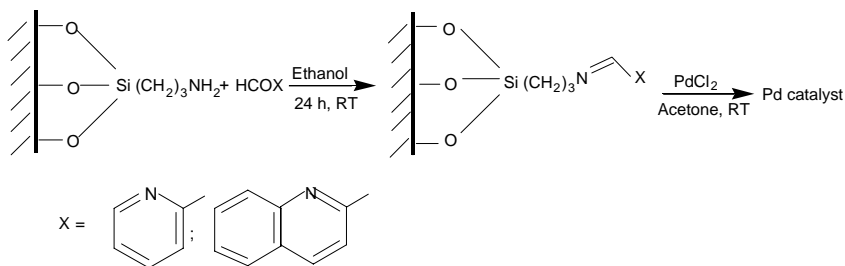


**Jana Horniakova, Thirumalaiswamy Raja,  
Yoshihiro Kubota, Yoshihiro Sugi**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 73

Pyridine-derived palladium complexes immobilized on ordered mesoporous silica as catalysts for Heck-type reactions

Palladium complexes immobilized on pyridine–carboimine and quinoline–carboimine functionalized mesoporous FSM-16 were prepared and applied for the Heck vinylation and the Suzuki coupling of aryl bromides as active and re-usable catalysts.

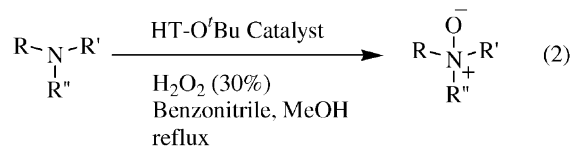
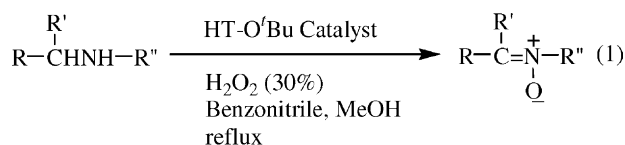


**B.M. Choudary, Ch. Venkat Reddy,  
B. Veda Prakash, B. Bharathi,  
M. Lakshmi Kantam**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 81

Oxidation of secondary and tertiary amines by a solid base catalyst

The catalytic oxidation of *sec*- and *tert*-amines to nitrones (Eq. (1)), amine *N*-oxides (Eq. (2)), respectively, is realised by HT-O<sup>t</sup>Bu catalyst, and benzonitrile as an additive, using 30% hydrogen peroxide at a faster rate in quantitative yields. The catalyst is reused for five recycles without significant loss of activity and selectivity.

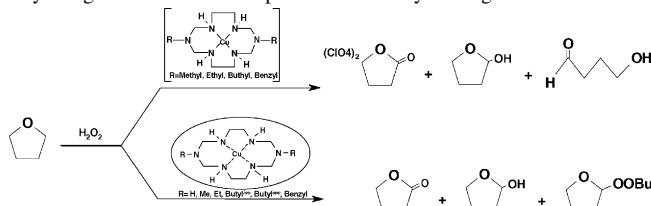


**Masoud Salavati-Niasari**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 87

Zeolite-encapsulation copper(II) complexes with 14-membered hexaaza macrocycles: synthesis, characterization and catalytic activity

Copper(II) complexes with 14-membered hexaaza macrocyclic ligand “1,3,6,8,10,13-hexaazacyclotetradecane” “[Cu(R<sub>2</sub>[14]aneN<sub>6</sub>)](ClO<sub>4</sub>)<sub>2</sub> R = Me, Et, Bu, benzyl” have been prepared by the one-pot template reactions of formaldehyde and ethylenediamine with alkyl and benzyl amine within the cavities of zeolite Y “[CuR<sub>2</sub>[14]aneN<sub>6</sub>]-NaY”. The new materials were characterized by several techniques: chemical analysis and spectroscopic methods (FT-IR, UV-Vis, XRD, BET, DRS). By comparing the performance of the heterogeneous system with the neat complex in the oxidation of tetrahydrofuran (THF) using hydrogen peroxide as oxygen donor, a protection effect of the matrix over the active center was evidenced by a higher conversion and product selectivity are higher.

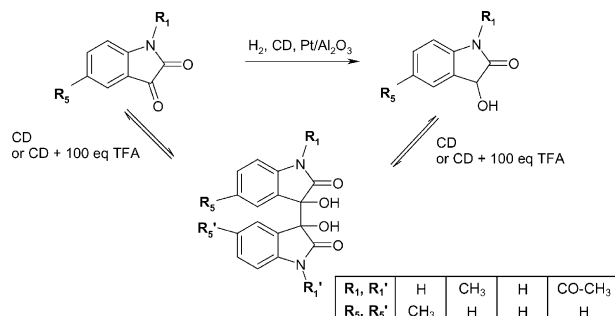


**Otmar J. Sonderegger, Thomas Bürgi,  
Ludwig K. Limbach, Alfons Baiker**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 93

Enantioselective reduction of isatin derivatives over cinchonidine modified Pt/alumina

The asymmetric hydrogenation of isatin and its derivatives leads at low CD concentration to the corresponding alcohol, at high CD concentration or CD and 100 eq. TFA to the corresponding isatide (CD: cinchonidine).

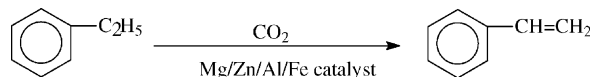


**Xingnan Ye, Ning Ma, Weiming Hua,  
Yinghong Yue, Changxi Miao, Zaiku Xie,  
Zi Gao**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 103

Dehydrogenation of ethylbenzene in the presence of CO<sub>2</sub> over catalysts prepared from hydrotalcite-like precursors

Dehydrogenation of ethylbenzene in the presence of CO<sub>2</sub> over Fe-containing mixed oxide catalyst prepared from hydrotalcite-like precursors is reported. Mg/Zn/Al/Fe catalyst affords an ethylbenzene conversion of 53.8% and a styrene selectivity of 96.7% at 773 K.

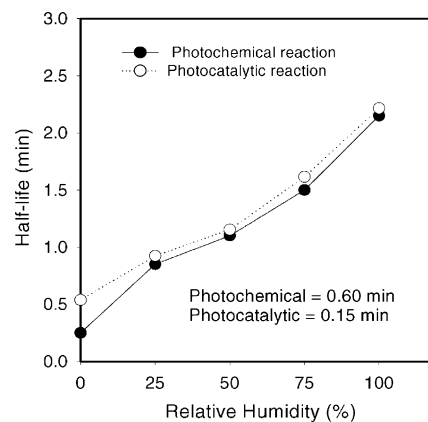


**Placidus B. Amama, Kiminori Itoh,  
Masayuki Murabayashi**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 109

Photocatalytic degradation of trichloroethylene in dry and humid atmospheres: role of gas-phase reactions

The optimum relative humidity for photocatalytic degradation of trichloroethylene is ~25% because high reactivity and degradation of trichloroethylene (TCE) to CO<sub>2</sub> are achieved simultaneously.

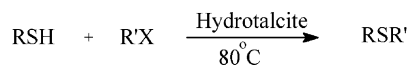


**Sakthivel Vijaikumar, Kasi Pitchumani**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 117

Simple, solvent free syntheses of unsymmetrical sulfides from thiols and alkyl halides using hydrotalcite clays

A wide range of unsymmetrical sulfides have been synthesized in good yield from thiols and alkyl halides using synthetic hydrotalcite clays as basic catalysts.



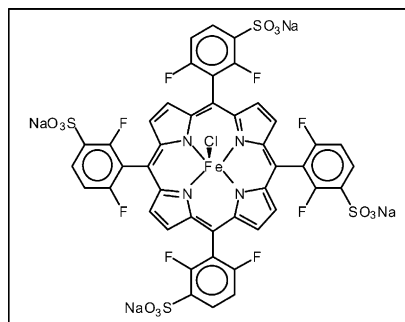
R = C<sub>6</sub>H<sub>5</sub>, *p*-Cl-C<sub>6</sub>H<sub>4</sub>, *p*-CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>, n-butyl, n-hexyl or n-octyl  
R' = allyl, n-propyl, isopropyl, n-butyl or benzyl  
X = Br, Cl or I

**Shirley Nakagaki, Flávio Luiz Benedito,  
Fernando Wypych**

*Journal of Molecular Catalysis A: Chemical* 217  
(2004) 121

Anionic iron(III) porphyrin immobilized on silanized kaolinite as catalyst for oxidation reactions

Silanized kaolinite was used as a new inorganic support for immobilization of the anionic iron(III) porphyrin [(FeTDFSP)Cl]<sup>4-</sup>. The material (kaolinite-iron(III) porphyrin) was an efficient and selective catalyst for oxidation reactions.

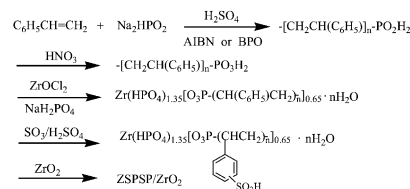


**Yan Sui, Xiangkai Fu, Renquan Zeng, Xuebing Ma**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 133

Preparation, characterization and application of a new type of ion exchanger and solid acid zirconium sulfonated oligo-polystyrenylphosphonate-phosphate supported on  $ZrO_2$

A new type of ion exchanger and solid acid zirconium sulfonated oligo-polystyrenyl phosphonate-phosphate supported on  $ZrO_2$  (ZSPSP/ $ZrO_2$ ) has been prepared, characterized by IR, SEM, TG and DSC and their acid catalytic and ion exchange properties has also been investigated.

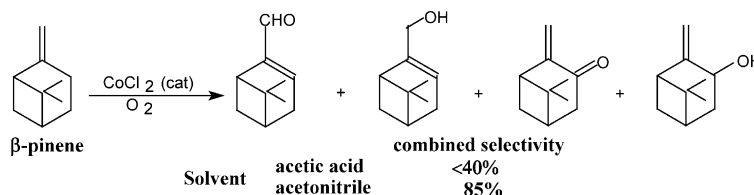


**Patricia A. Robles-Dutenhefner, Márcio J. da Silva, Luciana S. Sales, Edesia M.B. Sousa, Elena V. Gusevskaya**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 139

Solvent-free liquid-phase autoxidation of monoterpenes catalyzed by sol-gel  $Co/SiO_2$

A novel selective  $CoCl_2$  catalyzed oxidation of  $\beta$ -pinene in acetonitrile solutions resulting in allylic oxygenated derivatives has been developed. In acetic acid, the reaction is complicated by the substrate isomerization and acetic acid addition. Limonene and  $\alpha$ -pinene give both allylic oxidation and epoxidation products (molar ratio  $\approx 1/1$ ), with chemoselectivities being higher in acetonitrile than those in acetic acid.

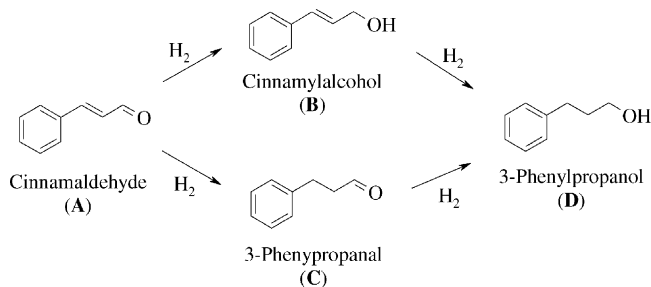


**Jan Hájek, Narendra Kumar, Päivi Mäki-Arvela, Tapio Salmi, Dmitry Yu. Murzin**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 145

Selective hydrogenation of cinnamaldehyde over Ru/Y zeolite

Selectivity in liquid-phase hydrogenation of cinnamaldehyde (A) to unsaturated alcohol cinnamylalcohol (B) over 5%Ru/Y-zeolite was seen to be substantially dependent on the reaction parameters, in particular the nature of solvent.

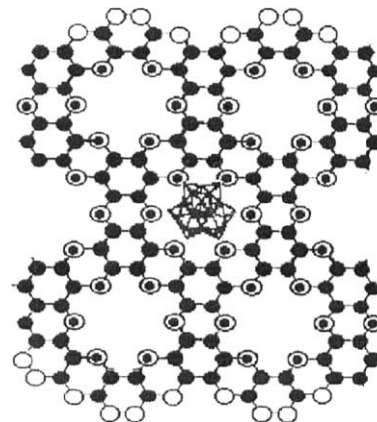


**M.N. Timofeeva, A.B. Ayupov, V.N. Mitkin, A.V. Volodin, E.B. Burgina, A.L. Chuvilin, G.V. Echevsky**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 155

New fluorinated carbon support for catalysts

The adsorption of  $H_3PW_{12}O_{40}$  from water and organic solvents by carbon meso-porous materials (Sibunit and fluorinated Sibunit (F-Sibunit)) was studied. A correlation between the rate constant of cyclohexene dimerisation of in the hexane solution and the strength of HPA-support interaction was determined.

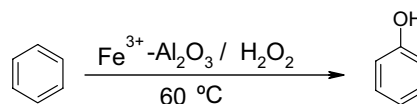


**Hassan Hosseini Monfared, Zahra Amouei**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 161

Hydrogen peroxide oxidation of aromatic hydrocarbons by immobilized iron(III)

Supported iron(III) ions on  $\gamma$ -alumina are an efficient catalyst for the oxidation of aromatic hydrocarbons with hydrogen peroxide in acetonitrile at 60 °C.

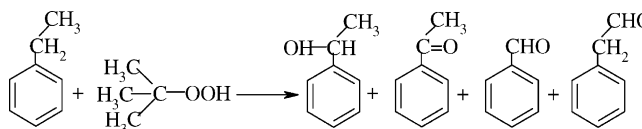


**S. Vetrivel, A. Pandurangan**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 165

Side-chain oxidation of ethylbenzene with *tert*-butylhydroperoxide over mesoporous Mn-MCM-41 molecular sieves

The liquid phase oxidation of ethylbenzene with *tert*-butylhydroperoxide was carried out over Mn-MCM-41 (29), Mn-MCM-41 (56), Mn-MCM-41 (73) and Mn-MCM-41 (104) gave  $\alpha$ -phenylethanol, acetophenone, benzaldehyde and phenyl acetaldehyde. Co-ordination of *tert*-butylhydroperoxide on Mn(II) is the essential for oxidation. The activity of the catalyst followed the order of Mn-MCM-41 (29) > Mn-MCM-41 (56) > Mn-MCM-41 (73) > Mn-MCM-41 (104).

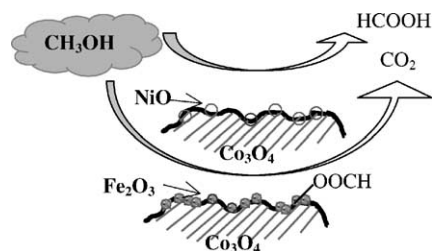


**Marta Maria Natile, Antonella Glisenti**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 175

Surface reactivity of NiO/Co<sub>3</sub>O<sub>4</sub> and Fe<sub>2</sub>O<sub>3</sub>/Co<sub>3</sub>O<sub>4</sub> nanocomposite catalysts: interaction with methanol

The interaction of NiO/Co<sub>3</sub>O<sub>4</sub> and Fe<sub>2</sub>O<sub>3</sub>/Co<sub>3</sub>O<sub>4</sub> with methanol was studied. HCOOH forms (RT) on the surface of both samples. CO<sub>2</sub> is also evident. Formate species are present on Fe<sub>2</sub>O<sub>3</sub>/Co<sub>3</sub>O<sub>4</sub>.

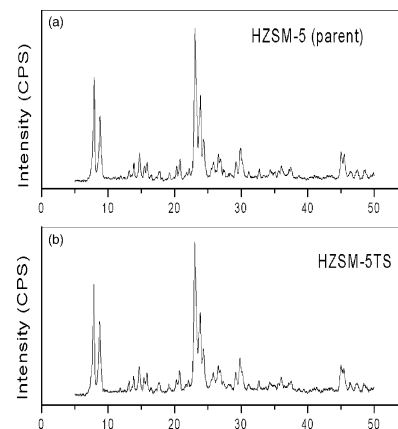


**N. Sharanappa, S. Pai, V.V. Bokade**

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 185

Selective alkylation and disproportionation of ethylbenzene in the presence of other aromatics

The interaction of NiO/Co<sub>3</sub>O<sub>4</sub> and Fe<sub>2</sub>O<sub>3</sub>/Co<sub>3</sub>O<sub>4</sub> with methanol was studied. HCOOH forms (RT) on the surface of both samples. CO<sub>2</sub> is also evident. Formate species are present on Fe<sub>2</sub>O<sub>3</sub>/Co<sub>3</sub>O<sub>4</sub>.

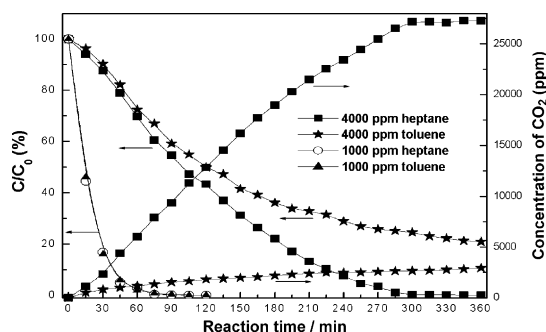


Chao Xie, Zili Xu, Qiuqing Yang, Na Li, Defeng Zhao, Debao Wang, Yaoguo Du

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 193

Comparative studies of heterogeneous photocatalytic oxidation of heptane and toluene on pure titania, titania-silica mixed oxides and sulfated titania

The photocatalytic degradation of heptane and toluene over UV-illuminated titania, titania-silica mixed oxides and sulfated titania was compared, and the deactivation and regeneration behavior of those three catalysts were investigated.

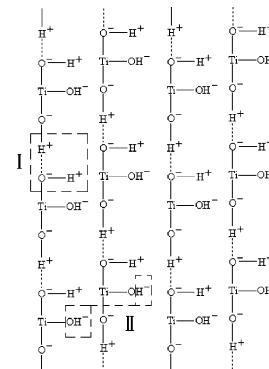


Min Zhang, Zhensheng Jin, Jingwei Zhang, Xinyong Guo, Jianjun Yang, Wei Li, Xiaodong Wang, Zhijun Zhang

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 203

Effect of annealing temperature on morphology, structure and photocatalytic behavior of nanotubed  $H_2Ti_2O_4(OH)_2$

Nanotubed  $H_2Ti_2O_4(OH)_2$  is thermally unstable and its dehydration consists of two steps: (i) dehydration of intralayered OH groups at  $T \leq 300^\circ C$ ; (ii) dehydration of interlayered OH groups at  $T > 300^\circ C$ .

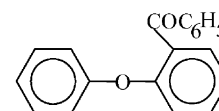
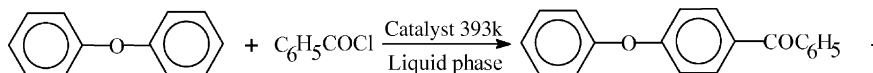


Dhanashri P. Sawant, Biju M. Devassy, S.B. Halligudi

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 211

Friedel-Crafts benzylation of diphenyl oxide over zirconia supported 12-tungstophosphoric acid

Liquid phase benzylation of diphenyl oxide (DPO) with benzoyl chloride (BC) was catalyzed by TPA/ $ZrO_2$  to give 4-(benzoyl) diphenyl oxide (97.4%) under optimized reaction conditions.



Xueqin Wang, Gongliang Li, Umit S. Ozkan

*Journal of Molecular Catalysis A: Chemical* 217 (2004) 219

Hydrogenation of hexanal over sulfided Ni-Mo/ $\gamma$ - $Al_2O_3$  catalysts

Hydrogenation of hexanal to hexanol was studied over sulfided Ni-Mo catalysts supported on  $\gamma$ - $Al_2O_3$ . Characterizations of the oxide and sulfide forms of the catalysts were performed using XRD, XPS, TPD, DRIFTS, and TEM/EDX techniques. The relationship between the molybdena surface coverage and the density of surface hydroxyl groups and their correlation with  $CO_2$  adsorption sites have been investigated. A strong correlation was observed between the selectivity of the catalysts towards heavy products, such as dimers, trimers and acetals and  $CO_2$  adsorption sites.

