

## Contents

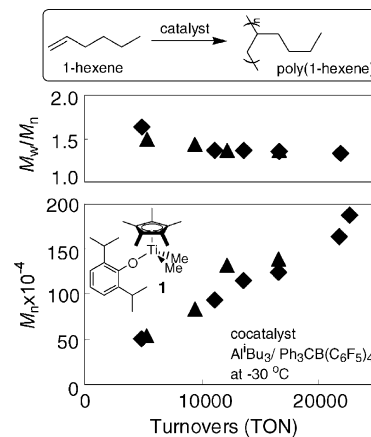
### Articles

**Kotohiro Nomura, Aya Fudo**

*Journal of Molecular Catalysis A: Chemical 209 (2004) 9*

Efficient living polymerization of 1-hexene by  $\text{Cp}^*\text{TiMe}_2(\text{O}-2,6\text{-}i\text{-Pr}_2\text{C}_6\text{H}_3)$ -borate catalyst systems at low temperature

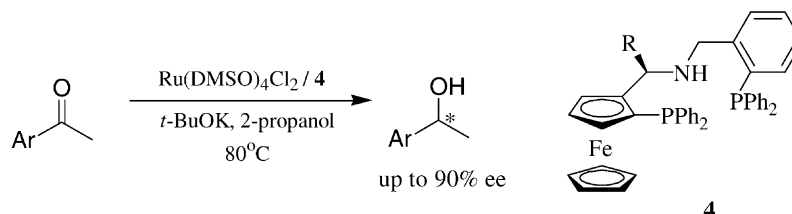
1-Hexene polymerization by  $\text{Cp}^*\text{TiMe}_2(\text{O}-2,6\text{-}i\text{-Pr}_2\text{C}_6\text{H}_3)$  (**1**) in the presence of  $\text{Ph}_3\text{CB}(\text{C}_6\text{F}_5)_4$  and  $\text{Al}^i\text{Bu}_3$  proceeded in a living manner at  $-30^\circ\text{C}$  with remarkably high catalyst efficiency, affording high molecular weight polymer with narrow polydispersity ( $M_n = 186.5 \times 10^4$ ,  $M_w/M_n = 1.27$ ). Effects of polymerization temperature, 1-hexene concentration, and Al cocatalyst were explored.



**Huicong Dai, Xiangping Hu, Huilin Chen, Changmin Bai, Zhuo Zheng**

*Journal of Molecular Catalysis A: Chemical 209 (2004) 19*

New chiral ferrocenyldiphosphine ligand for catalytic asymmetric transfer hydrogenation

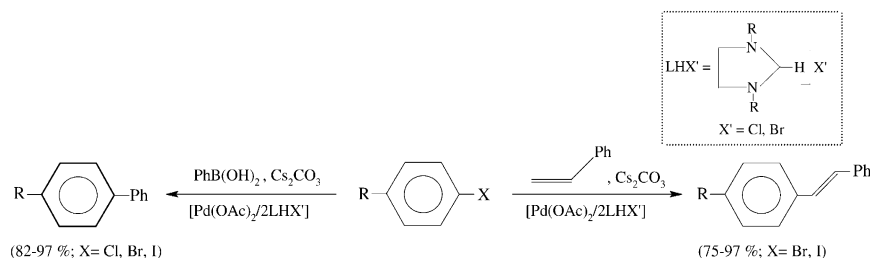


**Nevin Gürbüz, Ismail Özdemir, Serpil Demir, Bekir Çetinkaya**

*Journal of Molecular Catalysis A: Chemical 209 (2004) 23*

Improved palladium-catalyzed coupling reactions of aryl halides using saturated *N*-heterocarbene ligands

NHC complexes of Pd (II), in situ generated from  $\text{Pd}(\text{OAc})_2/2 \text{LHX}'$ , are found to be very active for Suzuki and Heck reactions: only, aryl chlorides are reluctant to give Heck coupling.

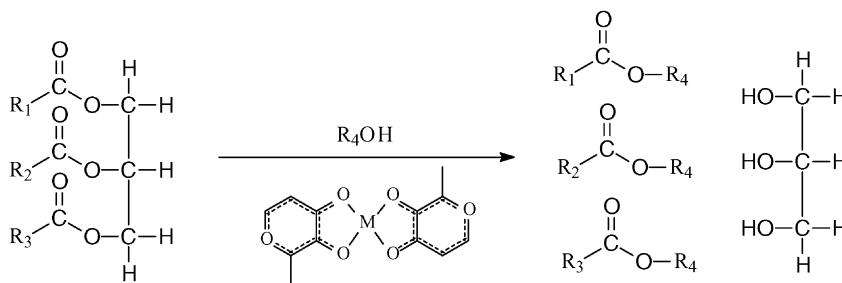


**Frederique R. Abreu, Daniella G. Lima,  
Elias. H. Hamú, Carlos Wolf, Paulo A.Z. Suarez**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 29

Utilization of metal complexes as catalysts in the transesterification of Brazilian vegetable oils with different alcohols

Sn(3-hydroxy-2-methyl-4-pyrone)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>, Pb(3-hydroxy-2-methyl-4-pyrone)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>, and Zn(3-hydroxy-2-methyl-4-pyrone)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> are seen to be active for different vegetable oils alcoholysis using different alcohols, including high molecular weight and branched ones.

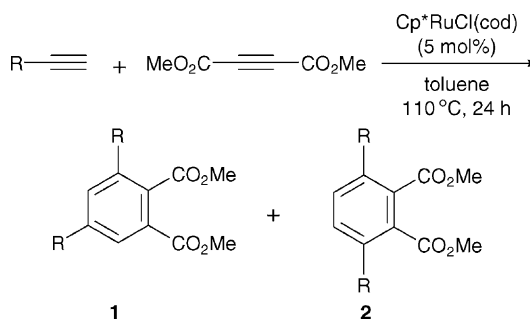


**Yasuyuki Ura, Yoshitaka Sato,  
Masashi Shiotsuki, Teruyuki Kondo,  
Take-aki Mitsudo**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 35

Ruthenium-catalysed synthesis of *o*-phthalates by highly chemoselective intermolecular [2 + 2 + 2] cycloaddition of terminal alkynes and dimethyl acetylenedicarboxylate

A highly chemoselective intermolecular [2 + 2 + 2] cycloaddition of 2 eq. of terminal alkynes with dimethyl acetylenedicarboxylate (DMAD), which enables the straightforward synthesis of *o*-phthalates, was successfully accomplished using a ruthenium catalyst, Cp<sup>\*</sup>RuCl(cod).

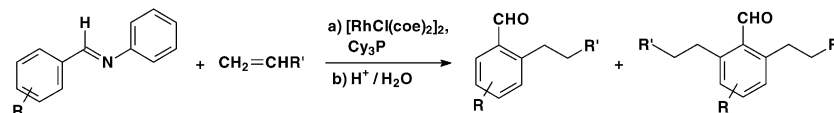


**Yeong-Gweon Lim, Jong-Soo Han,  
Bon Tak Koo, Jung-Bu Kang**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 41

Regioselective alkylation of aromatic aldimines and ketimines via C–H bond activation by a rhodium catalyst

The aldimines and ketimines reacted with alkenes under a rhodium catalyst [Rh(coe)<sub>2</sub>Cl]<sub>2</sub> and Cy<sub>3</sub>P to give mainly the double alkylated products with moderate to high yields. The aldimines bearing H, *p*-CH<sub>3</sub>O, *p*-CH<sub>3</sub>, *p*-Cl, *p*-F, *p*-CF<sub>3</sub> and *o*-CH<sub>3</sub> groups have high reactivities, but *m*-CH<sub>3</sub>O, *m*-Cl and *m*-F exhibit moderate reactivities. However, *o*-Cl, *o*-NO<sub>2</sub> and *p*-NO<sub>2</sub> groups did not work. The ketimine **9** gave the mono-alkylated products predominantly. 1-Naphthyl and heteroaromatic aldimines showed good regioselectivities.

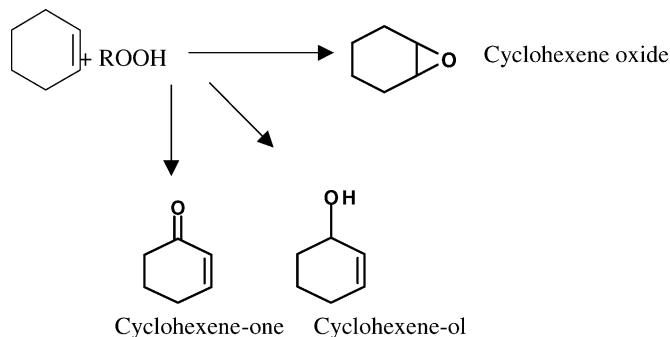


**Nthapo Sehlotho, Tebello Nyokong**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 51

Catalytic activity of iron and cobalt phthalocyanine complexes towards the oxidation of cyclohexene using *tert*-butylhydroperoxide and chloroperoxybenzoic acid

Catalytic oxidation of cyclohexene in the presence of iron and cobalt phthalocyanine complexes result in the formation of cyclohexene oxide, 2-cyclohexene-1-ol and 2-cyclohexene-1-one, with the selectivities of the products being dependant on the nature of the catalyst.



**László J. Csányi, Károly Jáky, Zoltán Kóta, Tibor Páli**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 59

Oxidation of hydrocarbons by O<sub>2</sub> in the presence of onium salts and onium ion-pair complexes as catalysts

Oxidations of cyclohexene and tetralin are induced by insertion of O<sub>2</sub> into activated C–H bonds. *N*-Onium salts catalyse the homolysis of these hydroperoxides into radicals. The catalytic activity is controlled by the partial charge of the cation, the polarizability of the counteranions and the concentration of the catalyst. The rate-influencing effects of the products and the activation parameters were determined, and the mechanism is outlined.

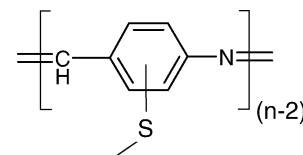


**Vendelín Macho, Milan Králik, Jozef Hudec, Jarmila Cingelova**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 69

One stage preparation of Schiff's bases from nitroarenes, aldehydes and carbon monoxide at presence of water

Using a sulfur-based catalytic system, nitroarenes, carbon monoxide and water react to the corresponding amines. In the presence of aldehydes, Schiff's bases are formed. Applying nitrocarbonyl compounds, e.g. 4-nitrobenzaldehyde, polymeric substances are obtained, in which sulfur acts as a cross-linker.

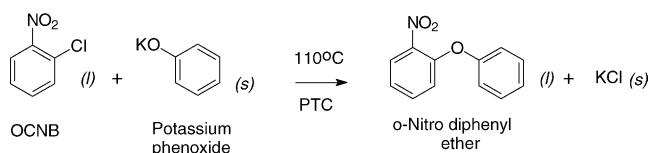


**Ganapati D. Yadav, S. Subramanian**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 75

Novelties of solid–liquid phase transfer catalyzed synthesis of *o*-nitrodiphenyl ether

The solid–liquid PTC reaction is 100% selective with very high rates of reactions vis-à-vis the liquid–liquid PTC process.

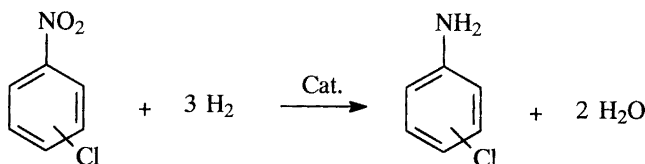


**Xiaoxiang Han, Renxian Zhou, Guohua Lai, Baohua Yue, Xiaoming Zheng**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 83

Effect of transition metal (Cr, Mn, Fe, Co, Ni and Cu) on the hydrogenation properties of chloronitrobenzene over Pt/TiO<sub>2</sub> catalysts

Selective hydrogenation of chloronitrobenzene to the corresponding chloroaniline has been studied in ethanol at 303 K and normal pressure over Pt/TiO<sub>2</sub> catalyst modified by transition metal (Cr, Mn, Fe, Co, Ni and Cu).

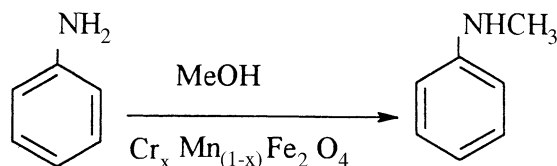


**K. Nishamol, K.S. Rahna, S. Sugunan**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 89

Selective alkylation of aniline to *N*-methyl aniline using chromium manganese ferrosinels

Vapour phase alkylation of aniline with methanol is done over  $\text{Cr}_x\text{Mn}_{1-x}\text{Fe}_2\text{O}_4$  ( $x = 0, 0.2, 0.4, 0.6, 0.8$  and 1.0) type ferrosinels systems. The acidity–basicity determination revealed that the samples possess greater amount of basic sites than acidic sites. All the ferrite samples proved to be selective and active for *N*-monoalkylation of aniline leading to *N*-methyl aniline. The catalytic activity of the samples is correlated well with their acid–base properties and on the cation distribution.

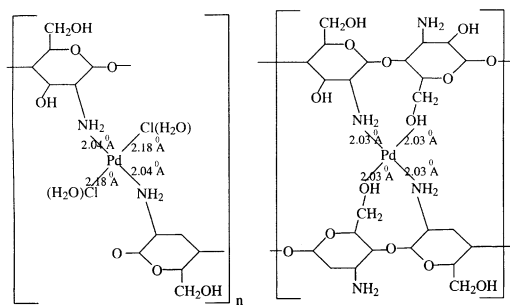


**Natalia V. Kramareva, Alexander Yu. Stakheev, Olga P. Tkachenko, Konstantin V. Klementiev, Wolfgang Grünert, Elena D. Finashina, Leonid M. Kustov**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 97

Heterogenized palladium chitosan complexes as potential catalysts in oxidation reactions: study of the structure

On the basis of IR and EXAFS investigations, it can be concluded that the structure of palladium complexes with chitosan depends on the preparation procedure. It was shown that reversible redox transformations of palladium immobilized on a chitosan matrix are possible.



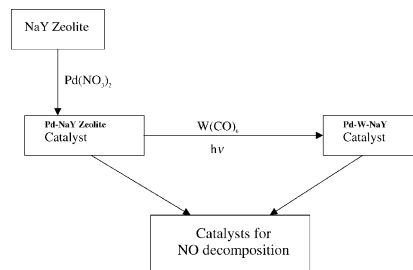
Adsorption chitosan-palladium complex Coprecipitated chitosan-palladium complex

**Sibele B.C. Pergher, Rogério M. Dallago, Renato Cataluña Veses, Carlos E. Gigola, Ione M. Baibich**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 107

Pd/NaY-zeolite and Pd-W/NaY-zeolite catalysts: preparation, characterization and NO decomposition activity

Pd/NaY-zeolite and Pd-W/NaY-zeolite catalysts were prepared from  $\text{Pd}(\text{NO}_3)_2$  and photochemical activation of  $[\text{W}(\text{CO})_6]$ . The catalysts were active for NO decomposition at 573 K leading mainly to  $\text{N}_2$  and  $\text{N}_2\text{O}$ . When the reduction pretreatment was 973 K the presence of tungsten led to higher conversion for a longer period of time. Tungsten prevents the sintering of small palladium particles and suppress  $\text{N}_2\text{O}$  formation.

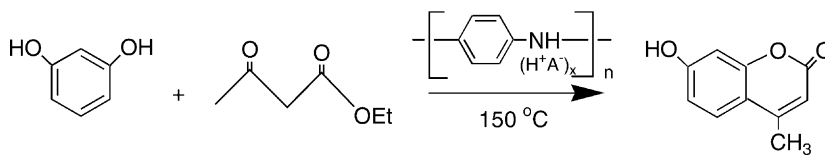


**Srinivasan Palaniappan, Rampally Chandra Shekhar**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 117

Synthesis of 7-hydroxy-4-methyl coumarin using polyaniline supported acid catalyst

Polyaniline-sulfate salts were prepared using four different oxidizing agents such as benzoyl peroxide, ammonium persulfate, sodium persulfate and potassium dichromate. Polyaniline-sulfate salts were characterized by spectral, physical and electrical methods. Polyaniline base was redoped to different polyaniline salts using various acids. Polyaniline salts are used as polymer supported acid catalysts for the preparation of 7-hydroxy-4-methyl coumarin. The catalytic use of polyaniline salts is feasible because of their easy preparation, stability, easy handling, less toxic, recovery, reusability and eco-friendly.

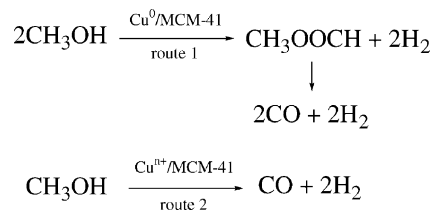


**T. Tsoncheva, Tz. Venkov, M. Dimitrov,  
C. Minchev, K. Hadjiivanov**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 125

Copper-modified mesoporous MCM-41 silica:  
FTIR and catalytic study

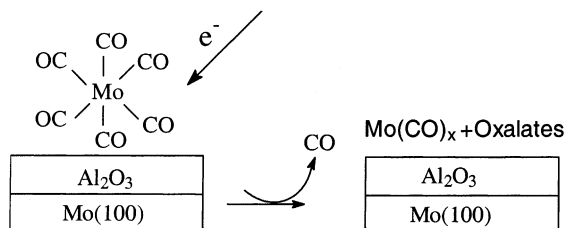
The participation of different copper species in the various methanol decomposition pathways is suggested. The regulation of their ratio by catalyst preparation could be a possible way for the methanol dehydrogenation selectivity control.



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

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 135

The effect of electron beam irradiation on the chemistry of molybdenum hexacarbonyl on thin alumina films in ultrahigh vacuum

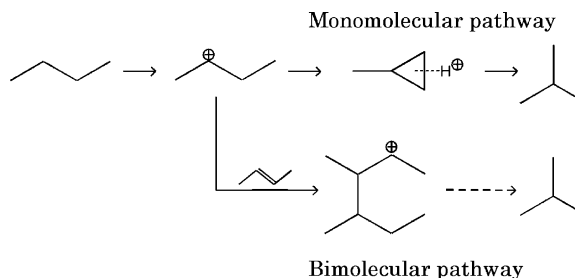


**Tsuneo Echizen, Tetsuo Suzuki, Yuichi Kamiya,  
Toshio Okuhara**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 145

Mechanistic study on skeletal isomerization of *n*-butane using  $1,4\text{-}^{13}\text{C}_2$ -*n*-butane on typical solid acids and their Pt-promoted bifunctional catalysts

On the solid acids, such as  $\text{Cs}_{2.5}\text{H}_{0.5}\text{PW}_{12}\text{O}_{40}$ , sulfated  $\text{ZrO}_2$ , and  $\text{WO}_3/\text{ZrO}_2$ , the isomerization of *n*-butane proceeded via a bimolecular pathway at low reaction temperatures and parallel (mono and bimolecular) pathways at high temperatures. In contrast, the monomolecular mechanism operated the reaction on Pt-promoted catalysts in the presence of  $\text{H}_2$  over the wide range of the reaction temperature.

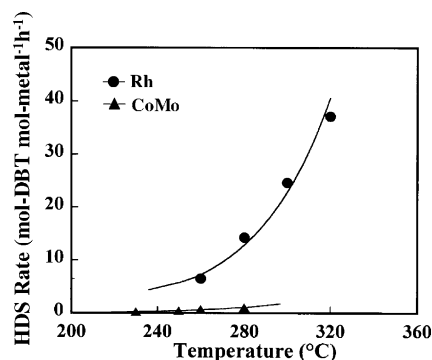


**Jeayoung Lee, Atsushi Ishihara,  
Franck Dumeignil, Kou Miyazaki,  
Yuji Oomori, Eika W. Qian, Toshiaki Kabe**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 155

Novel hydrodesulfurization catalysts derived from a rhodium carbonyl complex

Catalysts derived from alumina-supported rhodium carbonyl exhibited a higher DBT HDS activity than that of Ru carbonyl-based catalysts. Further, the specific activity calculated per rhodium was considerably higher than the one of a conventional Co-Mo catalyst. The high performances were explained by the formation of a great quantity of active sites (labile sulfur atoms).

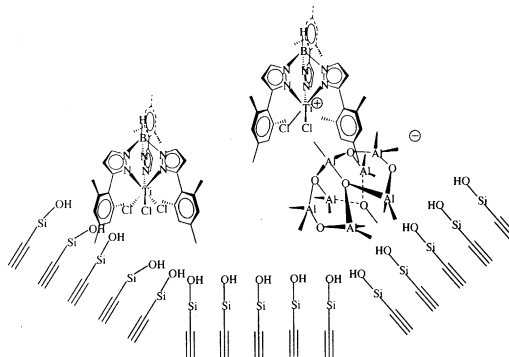


**Marcelo P. Gil, João H. Z. dos Santos,  
Osvaldo L. Casagrande Jr.**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 163

Polymerization of ethylene by the tris(pyrazolyl)-  
borate titanium(IV) compound immobilized on  
MAO-modified silicas

The immobilization of soluble catalyst  $\{\text{Tp}^{\text{Ms}^*}\}\text{TiCl}_3$  on silica and MAO-modified silicas containing 4.0, 8.0 and 23.0 wt.%  $\text{Al}/\text{SiO}_2$  and their use in ethylene polymerization are described.

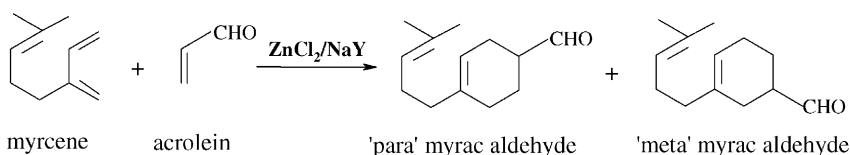


**Jianfu Liu, Donghong Yin, Dulin Yin,  
Zaihui Fu, Qianhe Li, Gongxuan Lu**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 171

$\text{ZnCl}_2$  supported on NaY zeolite by solid-state  
interaction under microwave irradiation and used  
as heterogeneous catalysts for high regioselective  
Diels–Alder reaction of myrcene and acrolein

$\text{ZnCl}_2/\text{NaY}$  catalyst prepared by a novel method of solid-state interaction between  $\text{ZnCl}_2$  and NaY zeolite under microwave irradiation is shown to catalyze efficiently the Diels–Alder reaction. Excellent catalytic activity and high regioselectivity of 'paralmeta' are achieved. The new Lewis acid sites formed on the surface of NaY zeolite are responsible for the high regioselective synthesis of 'para' myrac aldehyde.

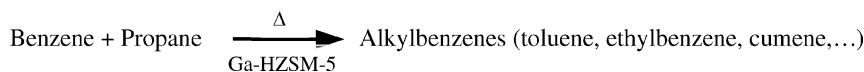


**C. Bigey, B.-L. Su**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 179

Propane as alkylating agent for alkylation of ben-  
zene on HZSM-5 and Ga-modified HZSM-5 zeo-  
lites

The product formation pathways of alkylation of benzene with propane on HZSM-5 and Ga-modified HZSM-5 suggest that acid-catalyzed cracking of propane predominates on HZSM-5, leading to the formation of toluene and ethylbenzene. Over Ga-modified HZSM-5, a bifunctional pathway is noted and cracking of propane and propane dehydrogenation are controlled by Lewis ( $\text{Ga}^{\text{x}+}$ )/Brønsted ( $\text{H}^+$ ) acid sites ratio.

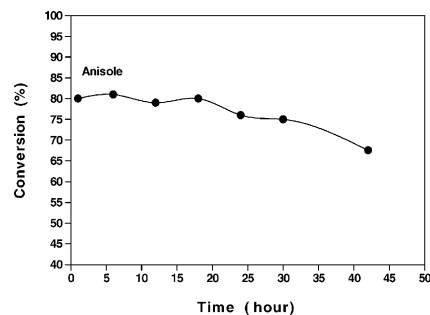


**Luiz A.M. Cardoso, Walter Alves. Jr.,  
Angélica R.E. Gonzaga, Leila M.G. Aguiar,  
Heloyza M.C. Andrade**

*Journal of Molecular Catalysis A: Chemical* 209  
(2004) 189

Friedel–Crafts acylation of anisole with acetic  
anhydride over silica-supported heteropolypho-  
sphotungstic acid (HPW/ $\text{SiO}_2$ )

The Friedel–Crafts acylation of anisole was investigated, using acetic anhydride and a silica-supported heteropolyphosphotungstic acid (HPW) catalyst. High conversion and selectivity were attained in the range of 61–110 °C. However, both a fast but reversible and a slower but irreversible deactivation of catalyst occurred, respectively, due to preferential adsorption of *p*-methoxyacetophenone and coking.

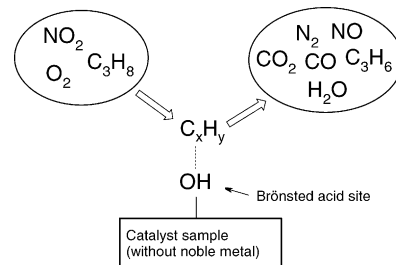


**Hanna Härelind Ingelsten, Åsa Hildesson,  
Erik Fridell, Magnus Skoglundh**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 199

The influence of surface acidity on NO<sub>2</sub> reduction by propane under lean conditions

This investigation focuses on the influence of the surface acidity on the continuous catalytic reduction of NO<sub>x</sub> by propane under lean conditions over alumina, silica and co-precipitated aluminium-silicates (without noble metals). The results indicate an increasing amount of Brønsted acid sites with increasing amount of alumina and the NO<sub>x</sub> reduction with propane correlates well with the Brønsted-site density.

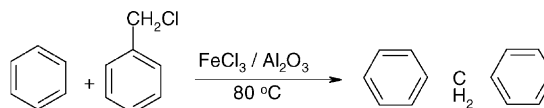


**M. Salavati-Niasari, J. Hasanalian, H. Najafian**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 209

Alumina-supported FeCl<sub>3</sub>, MnCl<sub>2</sub>, CoCl<sub>2</sub>, NiCl<sub>2</sub>, CuCl<sub>2</sub>, and ZnCl<sub>2</sub> as catalysts for the benzylation of benzene by benzyl chloride

Benylation of benzene in liquid phase by benzyl chloride to diphenylmethane over FeCl<sub>3</sub>, MnCl<sub>2</sub>, CoCl<sub>2</sub>, NiCl<sub>2</sub>, CuCl<sub>2</sub>, and ZnCl<sub>2</sub> supported on acidic alumina (at 80 °C) has been investigated. The supported FeCl<sub>3</sub> showed high conversion for the benzylation of benzene. The redox property of alumina-supported transition metal chloride seems to play a very important role in the benzene benzylation process.

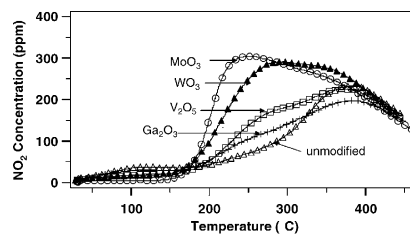


**Jazaer Dawody, Magnus Skoglundh,  
Erik Fridell**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 215

The effect of metal oxide additives (WO<sub>3</sub>, MoO<sub>3</sub>, V<sub>2</sub>O<sub>5</sub>, Ga<sub>2</sub>O<sub>3</sub>) on the oxidation of NO and SO<sub>2</sub> over Pt/Al<sub>2</sub>O<sub>3</sub> and Pt/BaO/Al<sub>2</sub>O<sub>3</sub> catalysts

This investigation focuses on the addition of metal oxides to barium-based NO<sub>x</sub> storage catalysts in order to increase their resistance against SO<sub>2</sub>. Addition of MoO<sub>3</sub> to Pt/Al<sub>2</sub>O<sub>3</sub> results in enhanced activity for NO oxidation and suppressed SO<sub>2</sub> oxidation rate in comparison with WO<sub>3</sub>, V<sub>2</sub>O<sub>5</sub>, Ga<sub>2</sub>O<sub>3</sub> modified or unmodified Pt/Al<sub>2</sub>O<sub>3</sub>. However, when MoO<sub>3</sub> is added to Pt/BaO/Al<sub>2</sub>O<sub>3</sub>, the NO<sub>x</sub> storage capacity during sulphur exposure declines faster than for unmodified Pt/BaO/Al<sub>2</sub>O<sub>3</sub> due to a faster decrease in the regeneration capacity during rich periods



Oxidation of NO over promoted Pt/Al<sub>2</sub>O<sub>3</sub> catalysts in presence of SO<sub>2</sub>

**Liang Li, Jianlin Shi, Jina Yan,  
Hongguang Chen, Xueguo Zhao**

*Journal of Molecular Catalysis A: Chemical* 209 (2004) 227

SBA-15 supported quaternary ammonium salt: an efficient, heterogeneous phase-transfer catalyst

The immobilization of an ammonium salt on the pore surface of highly hydrothermally stable inorganic mesoporous material SBA-15 provided an efficient phase-transfer catalyst that could easily be recovered and recycled.

