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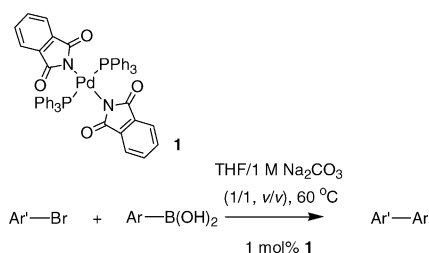
Articles

Nicholas M. Chaignon, Ian J.S. Fairlamb, Anant R. Kapdi, Richard J.K. Taylor, Adrian C. Whitwood

Journal of Molecular Catalysis A: Chemical 219 (2004) 191

Bis(triphenylphosphine)palladium(II)phthalimide – an easily prepared precatalyst for efficient Suzuki–Miyaura coupling of aryl bromides

The synthesis of a novel Pd(II) complex **1** containing a phthalimide ligand is reported. Its utility in the Suzuki–Miyaura coupling of aryl bromides with a variety of aryl- and heteroarylboronic acids, under relatively mild conditions, is described.

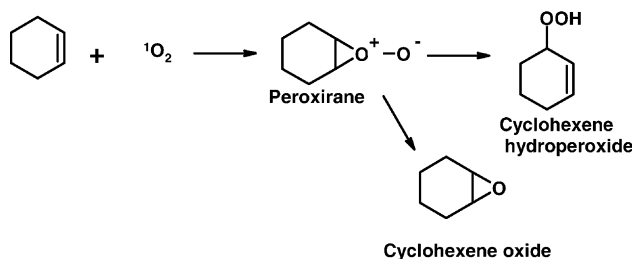


Nthapo Sehloho, Tebbello Nyokong

Journal of Molecular Catalysis A: Chemical 219 (2004) 201

Zinc phthalocyanine photocatalyzed oxidation of cyclohexene

Cyclohexene photooxidation catalyzed by zinc phthalocyanine resulted in the formation of cyclohexenone, cyclohexenol, *trans*-cyclohexanediol, cyclohexene oxide and cyclohexene hydroperoxide, through both singlet oxygen (Type II) and radical (Type I) mechanisms.

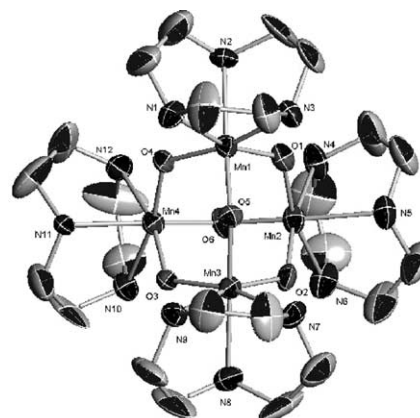


T.H. Bennur, D. Srinivas, S. Sivasanker, V.G. Puranik

Journal of Molecular Catalysis A: Chemical 219 (2004) 209

Catalytic activities of oxo–Mn–triazacyclononane complexes: spectral studies and single crystal X-ray structure of $[\text{Mn}_4\text{O}_6(1,4,7\text{-triazacyclononane})_4](\text{ClO}_4)_4 \cdot \text{H}_2\text{O}$

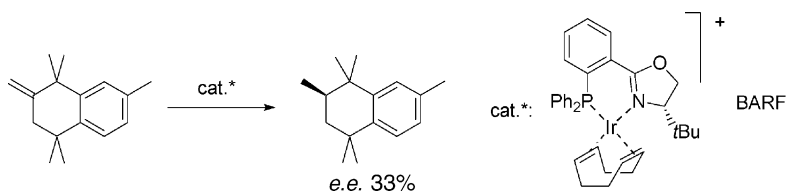
Monomeric terminal-oxo- and tetrameric bridged-oxo–Mn complexes viz., $[(\text{tmtacn})\text{Mn}(\text{O})(\text{H}_2\text{O})]\text{SO}_4$ and $[\text{Mn}_4\text{O}_6(\text{tacn})_4](\text{ClO}_4)_4 \cdot \text{H}_2\text{O}$, respectively, were isolated and characterized. Single crystal X-ray structure of the tetrameric bridged-oxo–Mn complex is reported. While the terminal-oxo–Mn complex exhibits efficient benzylic C–H bond oxidation activity of ethylbenzene with aqueous H_2O_2 as oxidant, the tetrameric bridged-oxo–Mn complex shows catalase activity. The study reveals the importance of nuclearity of the oxo–Mn species on the specific catalytic oxidation activity.



Alessandra Ciappa, Alberto Scrivanti,
Ugo Matteoli

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

The asymmetric hydrogenation of 1,1,4,4,7-pentamethyl-2-methylen-1,2,3,4-tetrahydro-naphthalene, a viable catalytic approach to the synthesis of non-racemic Fixolide[®]

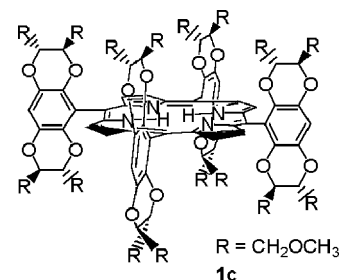


Hiroshi Nakagawa, Yoshihisa Sei,
Kentaro Yamaguchi, Tetsuo Nagano,
Tsunehiko Higuchi

Journal of Molecular Catalysis A: Chemical 219
(2004) 221

Catalytic and asymmetric epoxidation by novel D₄-symmetric chiral porphyrin derived from C₂-symmetric diol

Novel D₄-symmetric chiral porphyrin **1c** was efficiently prepared by utilizing C₂-symmetric diols as the chiral source. A symmetric epoxidation of aromatic olefins by **1c**-Fe(Br)/PhIO system showed moderate to high enantioselectivity.

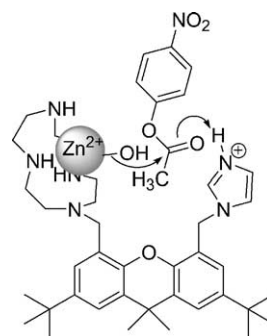


Neslihan Saki, Engin U. Akkaya

Journal of Molecular Catalysis A: Chemical 219
(2004) 227

Bifunctional catalysis of ester hydrolysis: novel hydrolytic enzyme models based on xanthenone framework

A bifunctional biomimetic catalyst accelerates the hydrolysis of a model substrate 5700-fold.



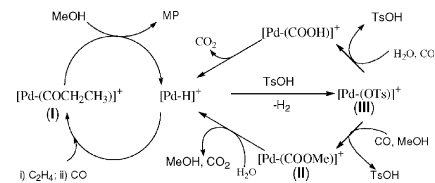
Gianni Cavinato, Luigi Toniolo,
Andrea Vavasori

Journal of Molecular Catalysis A: Chemical 219
(2004) 233

Characterization and catalytic activity of *trans*-[Pd(COCH₂CH₃)(TsO)(PPh₃)₂], isolated from the hydro-methoxycarbonylation of ethene catalyzed by [Pd(TsO)₂(PPh₃)₂]

The title complex (**I**) was isolated after the hydro-methoxycarbonylation (HMC) of ethene catalyzed by [Pd(TsO)₂(PPh₃)₂]. Also (**I**) is an active catalytic precursor (TOF = 420 h⁻¹ at 353 K, 4.5 MPa, CO/C₂H₄ = 1/1, Pd/PPh₃/TsOH = 1/8/10). At r.t., in MeOH saturated with CO, it gives methylpropanoate (MP) in stoichiometric amount and is converted to *trans*-[Pd(COOCH₃)(TsO)(PPh₃)₂] (**II**). (**II**) does not react with C₂H₄ in MeOH at r.t.; at 353 K, in the presence of *p*-toluenesulfonic acid (TsOH) and PPh₃, it is a precursor for the hydro-methoxycarbonylation, however is recovered as (**I**). The formation of (**I**), the conversion of (**I**) to (**II**) and of (**II**) to (**I**) are discussed in relation to the catalytic cycle, which is proposed to occur via a Pd(II)-H route,

through a type (**I**) intermediate. During catalysis, hydride consuming reactions occur with formation of (**II**) and/or [Pd(TsO)₂(PPh₃)₂], which are reconverted to the active hydride species upon interaction with CO and H₂O after CO₂ evolution.

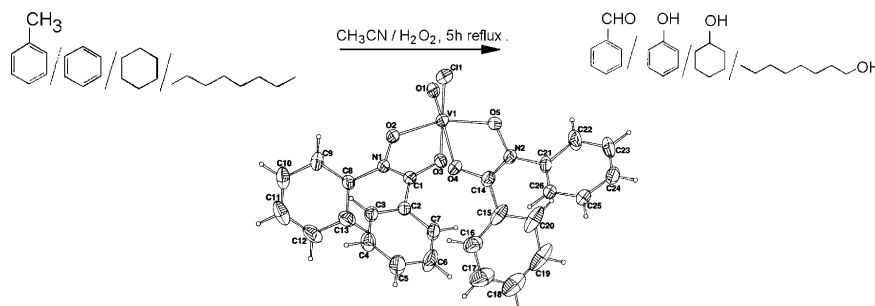


**Tapan K. Si, Krishna Chowdhury,
Monika Mukherjee, Dulal C. Bera,
Ramgopal Bhattacharyya**

Journal of Molecular Catalysis A: Chemical 219 (2004) 241

Homogeneous selective peroxidic oxidation of hydrocarbons using an oxovanadium based catalyst

Efficient selective hydrocarbon oxidation to their respective aldehydes, phenols, alcohols and ketones using H_2O_2 as terminal oxidant and oxovanadium(V) based catalyst.

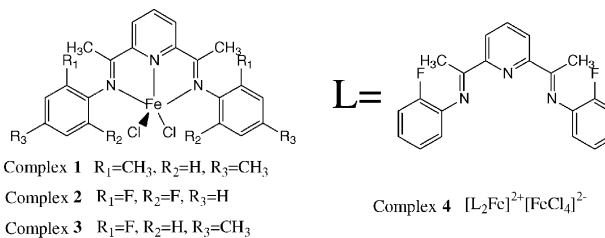


**Zhicheng Zhang, Junfeng Zou, Nannan Cui,
Yucai Ke, Youliang Hu**

Journal of Molecular Catalysis A: Chemical 219 (2004) 249

Ethylene oligomerization catalyzed by a novel iron complex containing fluoro and methyl substituents

A novel 2,6-bis(imino)pyridyl iron complex, $[2,6-(2\text{-F-4-CH}_3\text{C}_6\text{H}_3\text{N}=\text{CCH}_3)_2\text{C}_5\text{H}_3\text{N}]\text{FeCl}_2\cdot\text{H}_2\text{O}$ (**3**) has been synthesized and used for oligomerization of ethylene, which exhibit high catalytic activity ($>10^7$ g/molFe·h) and the products are mostly ($>90\%$) 1-butene, 1-hexene and 1-octene. Other three complexes (**1**, **2**, and **4**) are synthesized for comparison. The effects of substituents in the aryl rings and the reaction conditions on catalytic activities and product properties are discussed in detail.



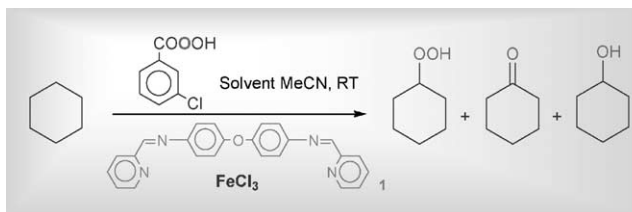
The structures of complexes 1-4

**Georgiy B. Shul'pin, Helen Stoeckli-Evans,
Dalmo Mandelli, Yuriy N. Kozlov,
Ana Tesouro Vallina, Camile B. Woitiski,
Ricardo S. Jimenez, Wagner A. Carvalho**

Journal of Molecular Catalysis A: Chemical 219 (2004) 255

Oxidation of alkanes with *m*-chloroperbenzoic acid catalyzed by iron(III) chloride and a polydentate amine

The addition to a metal-complex catalyst a polydentate amine (which mimics a peptide environment of a reaction center in enzymes) leads to a noticeable enhancement of the alkane oxidation rate as well as selectivity of the reaction.

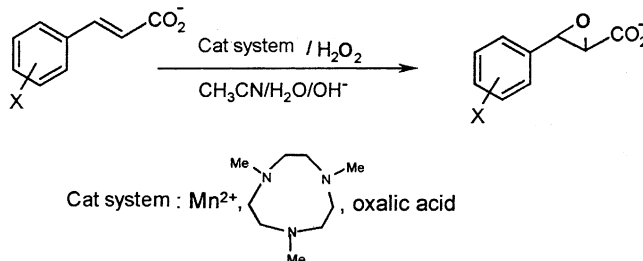


**Bruce C. Gilbert, John R. Lindsay Smith,
Antoni Mairata i Payeras, John Oakes,
Roger Pons i Prats**

Journal of Molecular Catalysis A: Chemical 219 (2004) 265

A mechanistic study of the epoxidation of cinnamic acid by hydrogen peroxide catalysed by manganese 1,4,7-trimethyl-1,4,7-triazacyclononane complexes

The influence of organic additives on the epoxidation of cinnamic acid by hydrogen peroxide, in the presence of Mn^{2+} and 1,4,7-trimethyl-1,4,7-triazacyclononane, has been studied. The most efficient system, with added oxalic acid, has been investigated in more detail and possible mechanisms for the reactions are presented.

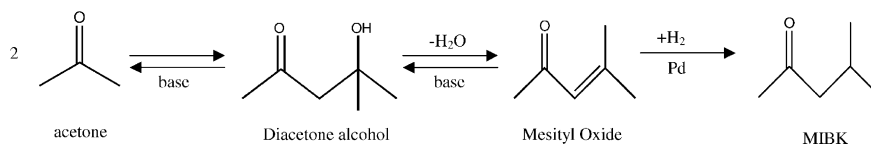


Ferry Winter, A. Jos van Dillen,
Krijn P. de Jong

Journal of Molecular Catalysis A: Chemical 219
(2004) 273

Single-stage liquid-phase synthesis of methyl isobutyl ketone under mild conditions

A catalyst mixture of activated Mg/Al hydrotalcite as solid base and Pd on carbon nanofibers was investigated for the synthesis of MIBK from acetone and hydrogen under mild conditions.

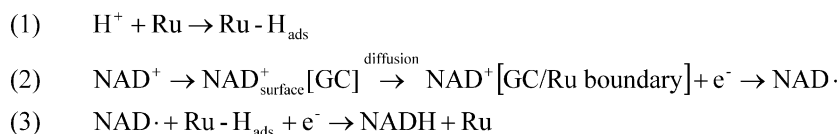


Amir Azem, Felise Man, Sasha Omanovic

Journal of Molecular Catalysis A: Chemical 219
(2004) 283

Direct regeneration of NADH on a ruthenium modified glassy carbon electrode

Regeneration of enzymatically active NADH on a Ru-modified GC electrode is promoted by the fast hydrogenation of NAD-radicals by hydrogen adsorbed on neighboring Ru nano-islands.

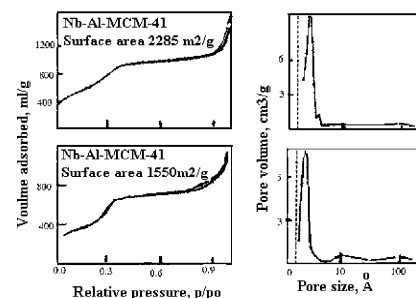


Deepak B. Akolekar, Suresh K. Bhargava

Journal of Molecular Catalysis A: Chemical 219
(2004) 301

Investigations on the novel niobium incorporated mesoporous catalytic materials

Novel niobium mesoporous (Nb-Al-MCM-41) catalysts with very high surface area (2285 m²/g) were synthesised and characterised. The catalysts were investigated for their NO/CO adsorption and disproportionation behaviour under various conditions.



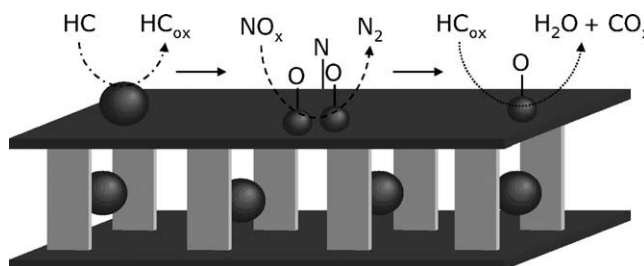
BET measurements over the niobium mesoporous catalysts

C. Belver, M.A. Vicente,
M. Fernández-García, A. Martínez-Arias

Journal of Molecular Catalysis A: Chemical 219
(2004) 309

Supported catalysts for DeNO_x reaction based on iron clays

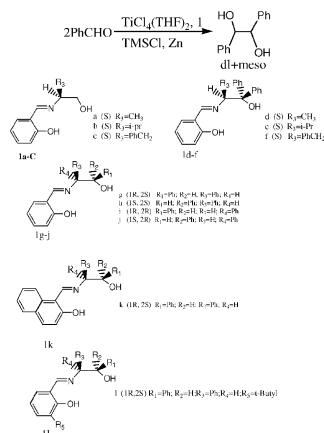
Iron species have been employed as active phase for the NO_x reduction with propene, choosing different modified clays as catalytic supports. The catalytic behaviour of the catalysts depends on the iron species, mainly located over the clay particles, and on the surface properties of the samples.



Qingshan Tian, Chen Jiang, Yougui Li, Changsheng Jiang, Tianpa You

Journal of Molecular Catalysis A: Chemical 219 (2004) 315

Experimental and theoretical investigation of the relationship between the steric structure of Schiff bases and the diastereoselectivity of pinacol produced from benzaldehyde

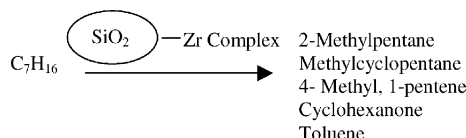


K.S. Anisia, A. Kumar

Journal of Molecular Catalysis A: Chemical 219 (2004) 319

Oxidation of *n*-heptane with molecular oxygen using heterogeneous catalyst formed by covalently binding [1,2-bis(salicylidene amino)-phenylene] zirconium complex to modified silica gel

Oxidation of *n*-heptane with molecular oxygen using heterogeneous catalyst formed by covalently binding [1,2-bis(salicylidene amino)-phenylene] zirconium complex to modified silica gel. Oxidation reactions of *n*-heptane were studied in presence of a heterogeneous catalyst consisting of [1,2-bis(salicylidene amino)-phenylene] zirconium complex chemically bonded to carbamate modified silica gel in the temperature range 160–220 °C.

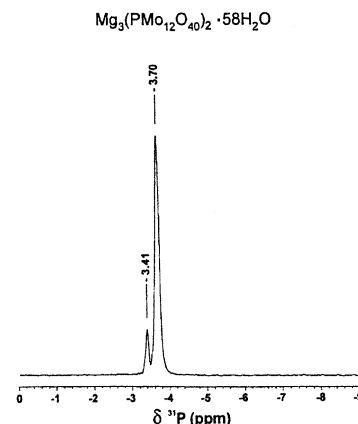


Eddy Silviani, Robert C. Burns

Journal of Molecular Catalysis A: Chemical 219 (2004) 327

Synthesis and characterization of soluble alkali metal, alkaline earth metal and related Keggin-type [PMo₁₂O₄₀]³⁻ salts for heterogeneous catalysis reactions

Soluble [PMo₁₂O₄₀]³⁻ salts containing the Group 1 (Li⁺ and Na⁺), Group 2 (Mg²⁺, Ca²⁺, Sr²⁺ and Ba²⁺) and Group 13 (Al³⁺) metals have been synthesized and thoroughly characterized by chemical analysis, TGA/DTA, IR spectroscopy, X-ray and neutron powder diffraction {Ba₃[P-Mo₁₂O₄₀]₂·(55.3)D₂O for the latter only}, and by both solid-state and solution ³¹P NMR spectroscopy.

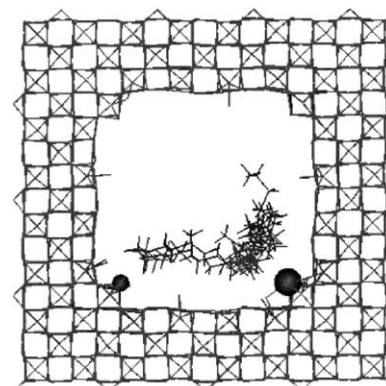


Bartłomiej Szyja, Jerzy Szczygieł

Journal of Molecular Catalysis A: Chemical 219 (2004) 343

Energetically preferred locations of hydrocarbons in the structure of a Pt-Sn/γ-Al₂O₃ catalyst: docking method

The most probable locations of hydrocarbon molecules on the micropore surface of a Pt-Sn/γ-Al₂O₃ catalyst were determined using the docking method. The results revealed a very strong influence of the platinum centres and a considerably weaker one of the tin centres, comparable to those of the support atoms. Aliphatic hydrocarbons adsorb much closer to the micropore surface than do cyclic hydrocarbons.

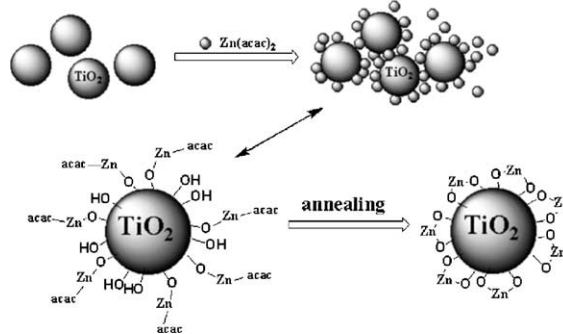


**Ji-Chuan Xu, Yan-Li Shi, Ji-Er Huang,
Bo Wang, Hu-Lin Li**

Journal of Molecular Catalysis A: Chemical 219
(2004) 351

Doping metal ions only onto the catalyst surface

A new method for doping metal ions onto the TiO_2 surface is reported. The surface-doped TiO_2 exhibits higher photocatalytic activity than pure TiO_2 for the degradation of methyl orange in water.



A.B. Gaspar, L.C. Dieguez

Journal of Molecular Catalysis A: Chemical 219
(2004) 357

Reduction and desorption with carbon monoxide in Cr/SiO_2 catalysts for ethylene polymerization

Cr^{3+} species modifies the reduction profiles of Cr^{6+} and CO desorption in Cr/SiO_2 catalysts. This effect was not verified in function of distinct $\text{Cr}_A^{2+}/\text{Cr}_B^{2+}$ ratios, obtained with different chromium precursors.

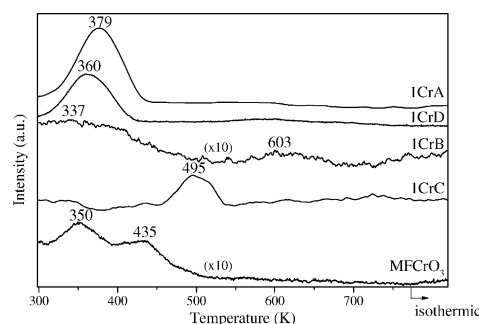


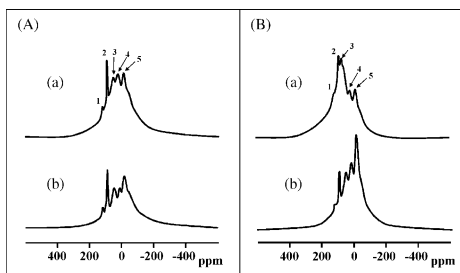
Figure. TPD profiles of CO for the catalysts and MFCr_2O_3 physical mixture

**Boping Liu, Keiji Fukuda, Hisayuki Nakatani,
Isa Nishiyama, Mikio Yamahiro,
Minoru Terano**

Journal of Molecular Catalysis A: Chemical 219
(2004) 363

^{27}Al MAS solid state NMR study on coordinative nature of alkyl-Al cocatalysts on a novel SiO_2 -supported Ziegler-Natta catalyst for controlled multiplicity of molecular weight distribution

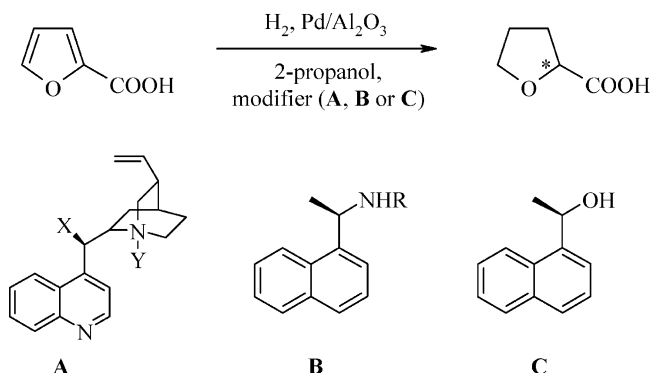
A novel SiO_2 -supported Ziegler-Natta catalyst with alkyl spacers on the surface was developed for ethylene polymerization. The catalyst showed unique catalytic properties for production of PE with significantly varied MWD by solely changing the types of cocatalyst. A good correlation between coordinative states of Al species on the activated catalysts and the MWD of PE was established by ^{27}Al MAS solid state NMR method.



**Mihaela Maris, Tamas Mallat,
Elisabeth Orglmeister, Alfons Baiker**

Journal of Molecular Catalysis A: Chemical 219
(2004) 371

On the role of modifier structure in the palladium-catalyzed enantioselective hydrogenation of furan-2-carboxylic acid

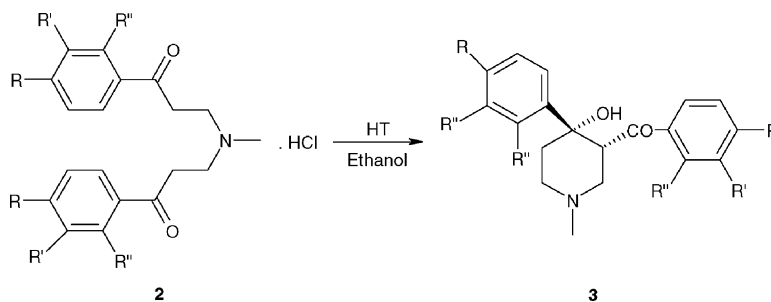


**Agnieszka Cwik, Aliz Fuchs, Zoltán Hell,
Jean-Marc Clacens**

Journal of Molecular Catalysis A: Chemical 219
(2004) 377

An efficient and environmental-friendly synthesis
of 4-hydroxy-arylpiperidines using hydrotalcite
catalyst

A practical and convenient synthesis of 4-hydroxy-arylpiperidines, starting from bis-ketonic Mannich-bases in the presence of a commercially available non-activated 2:1 Mg:Al hydrotalcite, is described.



Katalin Balázsik, Mihály Bartók

Journal of Molecular Catalysis A: Chemical 219
(2004) 383

Heterogeneous asymmetric reactions
Part 40. New data on repeated use of Pt-alumina
catalyst during enantioselective hydrogenation of
ethyl pyruvate

The repeated use of catalyst was studied under mild experimental conditions (H_2 : 1 bar, 253–298 K, [dihydrocinchonidine] = 0.001–0.1 mmol/l) in toluene and AcOH. In toluene an “increased in ee on reuse” was observed. This is an intrinsic feature of Pt-alumina-cinchona catalyst system, in which the restructuring of the Pt surface may play an important role.

