

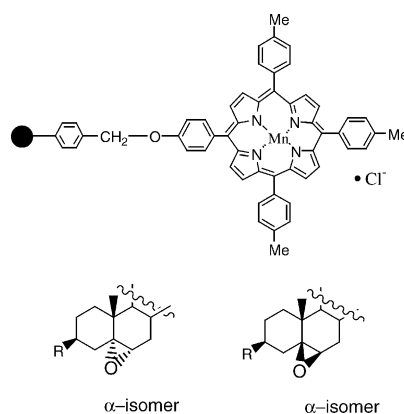
## Contents

### Articles

**Can-Ping Du, Zheng-Kai Li, Xiang-Min Wen,  
Jiang Wu, Xiao-Qi Yu, Meng Yang,  
Ru-Gang Xie**

*Journal of Molecular Catalysis A: Chemical 216  
(2004) 7*

Highly diastereoselective epoxidation of cholest-5-ene derivatives catalyzed by polymer-supported manganese(III) porphyrins

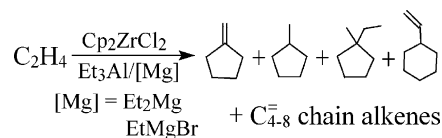


**Mei Wang, Dong Dai, Hongjun Zhu,  
Xiang Zhang, Licheng Sun**

*Journal of Molecular Catalysis A: Chemical 216  
(2004) 13*

Effects of the precatalyst structure and the Mg-containing third-component on cyclo-oligomerization of ethene

The catalytic cyclo-oligomerization of ethene by  $\text{Cp}_2\text{ZrCl}_2/\text{Et}_3\text{Al}/[\text{Mg}]$  ( $\text{Et}_2\text{Mg}$  or  $\text{EtMgBr}$ ) in a proper molar ratio of  $\text{Zr}/\text{Al}/\text{Mg}$  afforded *exo*-methylene-cyclopentane as major product. The other cyclic oligomers are methylcyclopentane, 1-methyl-1-ethylcyclopentane and vinylcyclohexane. The mechanism of the novel cyclo-oligomerization of ethene is discussed.

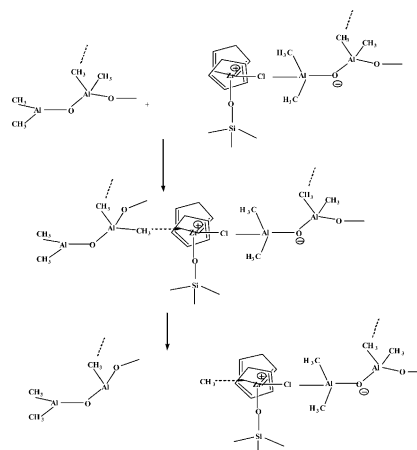


**Sílvia Rodrigues, Fernando Silveira,  
J.H.Z. dos Santos, M.L. Ferreira**

*Journal of Molecular Catalysis A: Chemical 216  
(2004) 19*

An explanation for experimental behavior of hybrid metallocene silica-supported catalyst for ethylene polymerization

JMCA “An explanation for experimental behavior of hybrid metallocene silica-supported catalyst for ethylene polymerization” Sílvia Rodrigues, Fernando Silveira, J.H.Z. dos Santos, M.L. Ferreira. This work presents the results of homopolymerization of ethylene using an hybrid system ( $n\text{BuCp}$ ) $_2\text{ZrCl}_2$ - $\text{Cp}_2\text{ZrCl}_2$ , soluble and supported on silica. The catalytic systems were analyzed by RBS, DRIFTS and EXAFS and polyethylenes (PE) by GPC and DSC. EHMO calculations allow us to conclude that  $\text{Cp}_2\text{ZrCl}_2$  has a strong affinity by AIS plane, whereas ( $n\text{BuCp}$ ) $_2\text{ZrCl}_2$  shows similar affinity for both silica planes. Formation of active site at surface.

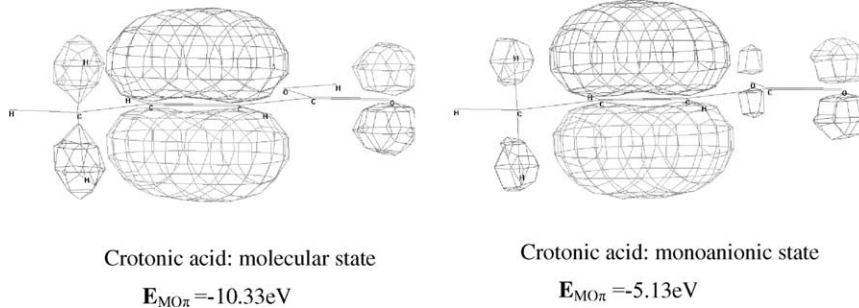


**Hong-chang Shi, Gang Chen, Xin-yan Wang, Zhi-guo Zhang**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 29

Epoxidation of  $\alpha$ ,  $\beta$ -unsaturated acids catalyzed by tungstate(VI) or molybdate (VI) in  $H_2O$ : influence of pH on epoxidation rate and a quantum chemical explanation

$E_{MO\pi}$  of  $\alpha$ ,  $\beta$ -unsaturated acid in monoanionic state is about 5 eV higher than that of in molecular state, which increase greatly the epoxidation reactivity of  $\pi$ -electrons in double bond.

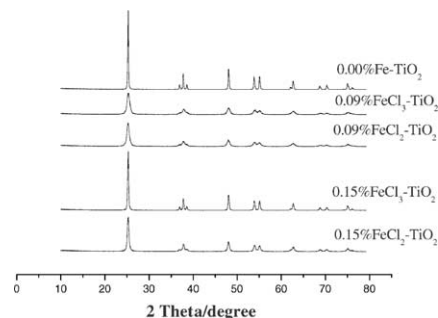


**Jiefang Zhu, Wei Zheng, Bin He, Jinlong Zhang, Masakazu Anpo**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 35

Characterization of Fe-TiO<sub>2</sub> photocatalysts synthesized by hydrothermal method and their photocatalytic reactivity for photodegradation of XRG dye diluted in water

Iron-ion-doped anatase titanium (IV) dioxide (TiO<sub>2</sub>) were prepared by hydrothermal method in this paper. Absorption, crystal size, specific surface area and photocatalytic activity of TiO<sub>2</sub> were obviously changed by doping. Iron doped with optimum content can enhance photocatalytic activity, especially under visible light irradiation.

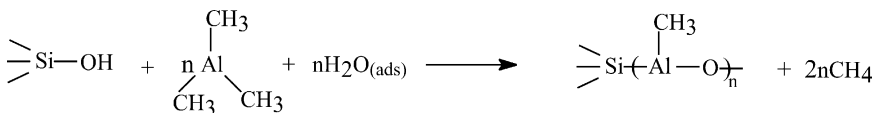


**Lílian Maria Tosta Simplício, Fábio Gomes Costa, Jaime Soares Boaventura, Emerson Andrade Sales, Soraia Teixeira Brandão**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 45

Study of some parameters on the zirconocene immobilization over silica

This work evaluates the effect of some parameters of the metallocene immobilization route in the ethylene polymerization. The results indicated that the route played an important role on the catalysts performance, polymer morphology and suggested the formation of MAO-like species on the silica surface from the reaction of TMA with water adsorbed or OH groups of the silica surface.

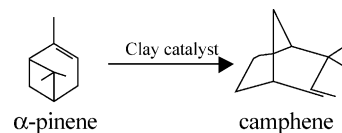


**Mukesh Kr. Yadav, Chintansinh D. Chudasama, Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 51

Isomerisation of  $\alpha$ -pinene using modified montmorillonite clays

Liquid phase catalytic isomerisation of  $\alpha$ -pinene with natural Indian Montmorillonite modified by sulphuric acid treatment and cation exchange was studied. More than 96%  $\alpha$ -pinene conversion is observed for acid treated clays with camphene selectivity ranging from 39 to 49%.

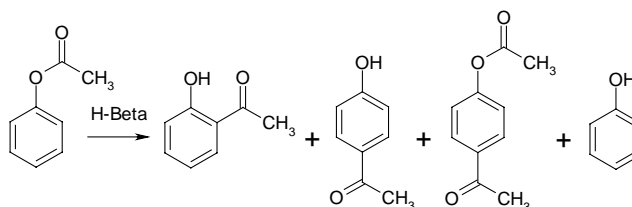


**E. Heitling, F. Roessner, E. van Steen**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 61

Origin of catalyst deactivation in Fries rearrangement of phenyl acetate over zeolite H-Beta

The zeolite catalysed Fries rearrangement of phenyl acetate: yielding *o*-HAP, *p*-HAP, *p*-AAP and phenol was investigated in a batch reactor. It is shown that the decline of activity of the catalyst in the initial period is associated with product inhibition by phenolic compounds (phenol and hydroxyacetophenons). The long-term deactivation is caused by coking.

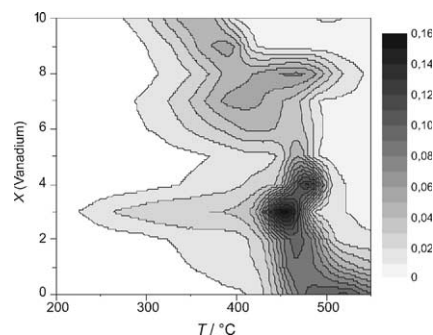


**Andreas H. Adams, Frank Haaß,  
Thorsten Buhrmester, Jan Kunert,  
Jörg Ott, Herbert Vogel, Hartmut Fuess**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 67

Structure and reaction studies on vanadium molybdenum mixed oxides

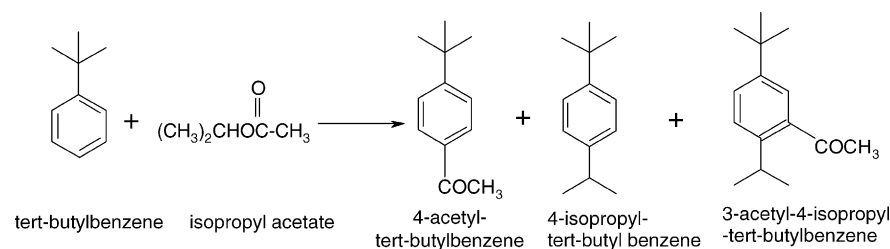
The correlation of the structure and the catalytic activity of vanadium molybdenum oxide catalysts were examined by X-ray diffraction and temperature programmed reduction measurements. The experiments revealed the presence of two metastable vanadium molybdenum mixed oxides,  $h$ -(V,Mo) $O_3$  and (V,Mo) $_2O_5$ , and an optimal vanadium molybdenum ratio of 3:7 for the yield of acrylic acid for acrolein.

**S. Udayakumar, A. Pandurangan, P.K. Sinha**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 75

Vapor phase reaction of tert-butylbenzene with isopropyl acetate over mesoporous Al-MCM-41 molecular sieves

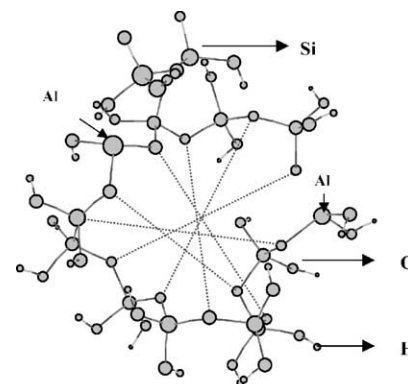
This work describes the Friedel–Crafts reaction of over tert-butylbenzene Al-MCM-41, using isopropyl acetate as an alkylating agent as well as an acylating agent in vapor phase. The reaction conditions for obtaining various products have been optimized by investigating their temperature, feed ratio, flow rate, and time-on-stream.

**G. Tonetto, M.L. Ferreira, H. de Lasa**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 83

Steam promoted mesoporosity in USY zeolites: structural properties and 1,2,4-TMB reactivity

This work addresses the potential effects of steaming in the case of dealumination of Y-zeolites. With this end, the interaction between 1,2,4-TMB and USY is analyzed. The zeolite is modeled using the complete exposed USY structure. MM2, PM3 and Extended Hückel methods are considered to evaluate the steric energies, changes in enthalpy and adsorption energies, upon 1,2,4-TMB adsorption and reaction on USY zeolite model.

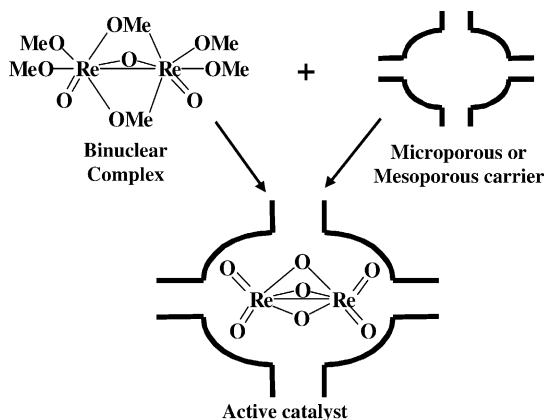


Reduced Window model for USY zeolite.

A.L. Kustov, V.G. Kessler, B.V. Romanovsky,  
G.A. Seisenbaeva, D.V. Drobot, P.A. Shcheglov

*Journal of Molecular Catalysis A: Chemical* 216  
(2004) 101

Supported Re and Mo oxides prepared using  
binuclear precursors: synthesis and characteriza-  
tion

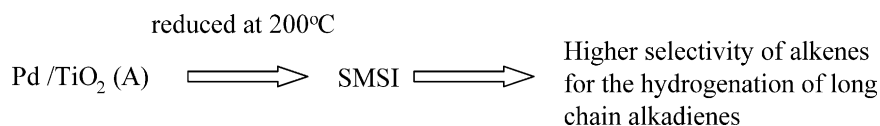


Yuanzhi Li, Bolian Xu, Yining Fan,  
Ninyuen Feng, Anding Qiu,  
Jianwen Miao, Jie He, Hanpei Yang, Yi Chen

*Journal of Molecular Catalysis A: Chemical* 216  
(2004) 107

The effect of titania polymorph on the strong  
metal-support interaction of Pd/TiO<sub>2</sub> catalysts  
and their application in the liquid phase selective  
hydrogenation of long chain alkadienes

The very different catalytic properties of Pd/TiO<sub>2</sub> (A) from Pd/TiO<sub>2</sub> (R) catalyst reduced at lower temperature is attributed to the presence of SMSI for Pd/TiO<sub>2</sub> (A) catalyst.

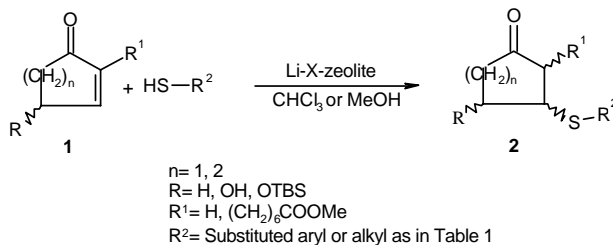


Popat D. Shinde, Vishal A. Mahajan,  
Hanumant B. Borate, Vasudha H. Tillu,  
Rajaram Bal, Asha Chandwadkar,  
Radhika D. Wakharkar

*Journal of Molecular Catalysis A: Chemical* 216  
(2004) 115

Li-X-type zeolite mediated Michael addition of  
thiols to cyclic enones and its application in the  
synthesis of 13-thiaprostaglandins

Michael addition of various thiols to cyclic enones in presence of Li-X-type zeolite has been described. 13-Thiaprostaglandins have been synthesized in good yields using substituted hydroxycyclopentenone as the Michael acceptor and arylthiols as Michael donors.

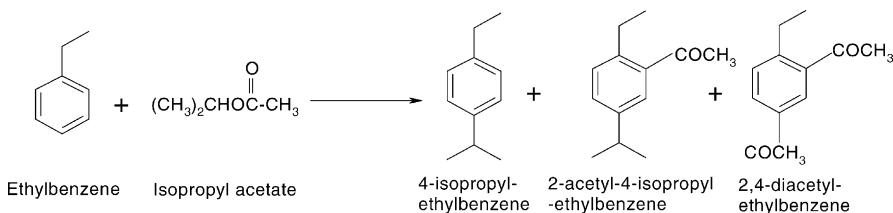


S. Udayakumar, A. Pandurangan, P.K. Sinha

*Journal of Molecular Catalysis A: Chemical* 216  
(2004) 121

Vapour phase reaction of ethylbenzene with iso-  
propyl acetate over mesoporous Al-MCM-41  
molecular sieves

This work describes the Friedel-Crafts reaction of ethylbenzene and isopropyl acetate over Al-MCM-41, possessing various types of acid sites. Isopropyl acetate is used as an alkylating agent as well as an acylating agent in vapour phase. The reaction conditions for obtaining various products have been optimised by investigating their temperature, feed ratio, flow rate and time on stream.

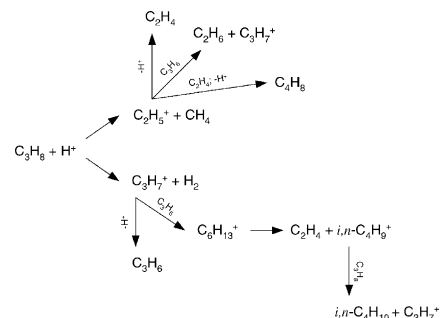


**X. Wang, H. Carabineiro, F. Lemos, M.A.N.D.A. Lemos, F. Ramôa Ribeiro**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 131

Propane conversion over a H-ZSM5 acid catalyst. Part 1. Observed kinetics

Propane conversion over H-ZSM5 zeolite follows two parallel reaction pathways: monomolecular cracking/dehydrogenation prevailing at high temperatures and low propane pressure involving pentacoordinated carbonium ions; bimolecular classical cracking through carbenium chain carriers is enhanced at low temperatures and high propane pressures. Dehydrogenation reactions are favored at low temperatures, while at higher temperatures cracking dominates.

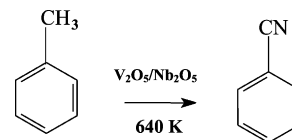


**Komandur V.R. Chary, Chinthala Praveen Kumar, Ayaluru Murali, Akhilesh Tripathi, Abraham Clearfield**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 139

Studies on catalytic functionality of  $V_2O_5/Nb_2O_5$  catalysts

The  $Nb_2O_5$  supported vanadium oxide catalyst is found to be highly active and selective for vapour phase ammoxidation of toluene. This paper provides information on the surface species and catalytic activity of  $Nb_2O_5$  supported vanadium oxide catalysts.

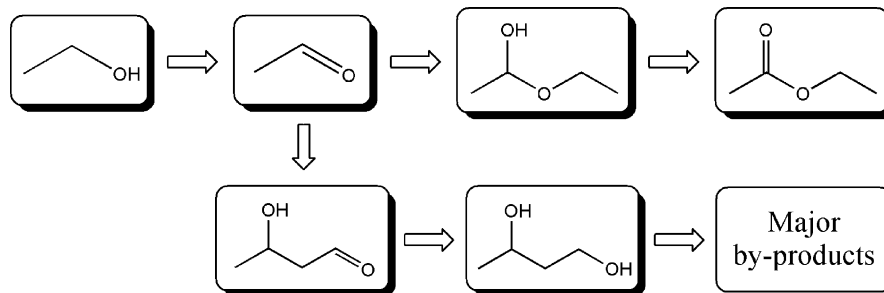


**Kanichiro Inui, Toru Kurabayashi, Satoshi Sato, Naoki Ichikawa**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 147

Effective formation of ethyl acetate from ethanol over Cu-Zn-Zr-Al-O catalyst

The major by-products in the direct synthesis of ethyl acetate from ethanol are formed by dehydration. Catalyst treatment with alkaline solution after reduction effectively suppressed formation of the by-products.



**M. Jhansi L. Kishore, G.S. Mishra, Anil Kumar**

*Journal of Molecular Catalysis A: Chemical* 216 (2004) 157

An alumina-supported homonuclear macrocyclic zirconium complex for reformation of *n*-hexane

A heterogenous formation catalyst supporting a homonuclear macrocyclic zirconium complex has been developed which reforms *n*-hexane at low temperature and pressure forming isomerized products.

