



## Contents

### Articles

**Fernando Ramo  Ribeiro, Jacques C. V drine**

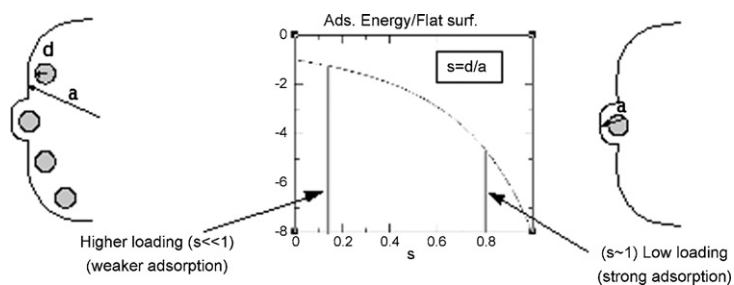
*Journal of Molecular Catalysis A: Chemical 305 (2009) 1*

In memory of our friend and colleague Eric Derouane, 1944–2008

**G. Sastre, A. Corma**

*Journal of Molecular Catalysis A: Chemical 305 (2009) 3*

The confinement effect in zeolites

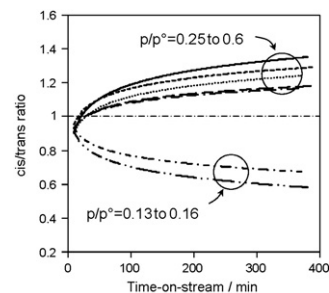


**Nathalie Tanchoux, St phane Pariente, Philippe Trems, Fran ois Fajula**

*Journal of Molecular Catalysis A: Chemical 305 (2009) 8*

Confinement and curvature effects as a tool for selectivity orientation in heterogeneous catalysis: Isomerisation of *n*-hexene over MCM-41-type catalysts

Confinement or curvature effects can significantly influence catalytic processes when using mesoporous catalysts. The isomerisation of 1-hexene into 2-hexene over MCM-41 catalysts under different 1-hexene partial pressures corresponding to those of the different sorption regimes is studied. Different reagent partial pressures (or sorption regimes) for a given pore size lead to a striking inversion of selectivity between the *cis*- and *trans*-2-hexene isomers.

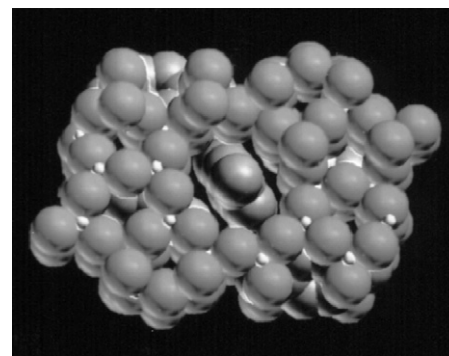


**A.A. Lucas, I. Derycke, Ph. Lambin, J.-P. Vigneron, L. Leherste, M. Elanany, J.-M. André, A.V. Larin, D.P. Vercauteren**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 16

Confinement in molecular sieves: The pioneering physical concepts

The aim of this contribution is to recall the pioneering physical concepts of confinement proposed by Eric Derouane, which have influenced more than 20 years of theoretical simulations of molecular sieves in Namur.

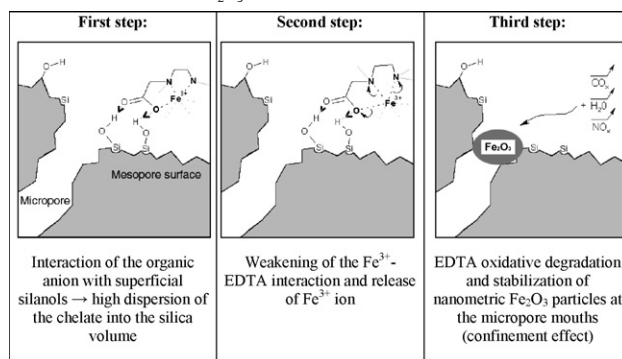


**S. Valange R. Palacio, A. Charmot, J. Barrault, A. Louati, Z. Gabelica**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 24

Nanoparticles of  $\text{Fe}_2\text{O}_3$  inserted in SBA-15 silica at micropore mouth level: An experimental evidence of the confinement effect

Mechanism illustrating schematically different steps of the thermal decomposition of  $\text{Fe}_2\text{O}_3/\text{SBA-15}$  composite synthesized using the chelate route, yielding nanosized  $\text{Fe}_2\text{O}_3$  particles confined at the micropore mouth levels inside the SBA-15 mesopores.

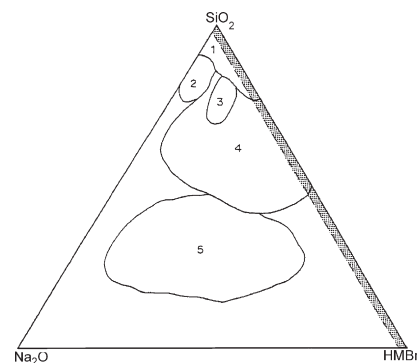


**G. Giordano, J.B. Nagy, E.G. Derouane**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 34

Zeolite synthesis in presence of hexamethonium ions

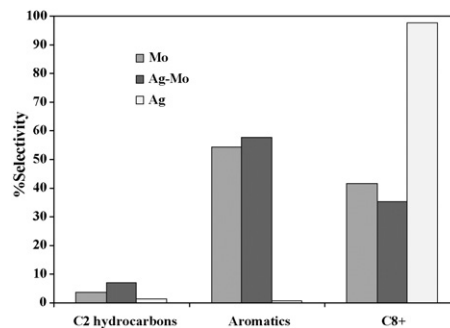
The role played by hexamethonium ions in the synthesis of one-dimensional ZSM-48 and EU-1 zeolitic structures is investigated. A systematic study is carried out to determine the factors influencing the preferential crystallization and/or co-crystallization of ZSM-48 and EU-1 from a sodium-hexamethonium-silica-alumina hydrogel. The influence of sodium and organic content and the Si/Al ratio in the initial hydrogel is specifically examined. An explanation is proposed for the accommodation of the hexamethonium ions in the different zeolitic frameworks of ZSM-48 and EU-1.



**M.W. Ngobeni, A.F. Carley, M.S. Scurrill, C.P. Nicolaides**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 40

The effects of boron and silver on the oxygen-free conversion of methane over Mo/H-ZSM-5 catalysts

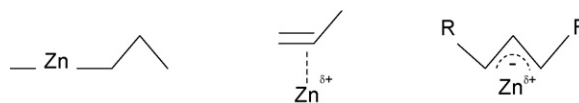


**Irina I. Ivanova, Yuriy G. Kolyagin,  
Vitaly V. Ordonsky, Ekaterina V. Asachenko,  
Elena M. Pasynkova, Yuri A. Pirogov**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 47

Surface species formed during propane aromatization over Zn/MFI catalyst as determined by in situ spectroscopic techniques

Propane aromatization has been studied in situ over Zn/H-MFI catalyst by  $^1\text{H}$ ,  $^{13}\text{C}$  MAS NMR and IR spectroscopic techniques. The following surface species were identified: (i) zinc propyl species; (ii) propene asymmetric  $\pi$ -complex with zinc cations; (iii) charge delocalized carbanionic species stabilized on zinc cations. The role of these species in the reaction pathway is discussed.

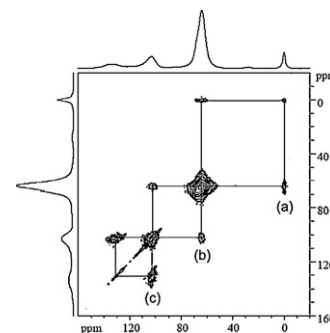


**Jean-Pierre Gilson, Christian Fernandez,  
Frédéric Thibault-Starzyk**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 54

New insights on zeolite chemistry by advanced IR and NMR characterization tools

New techniques and methodologies in spectroscopic characterization are yielding new insights in the complexity of zeolitic materials. Emerging IR and NMR techniques shed new lights on old problems such as acidity. New, rich and quantitative information can be gathered, with the ability to work under operando conditions. The work and inspiration of Eric Derouane are often at the core of this new knowledge.

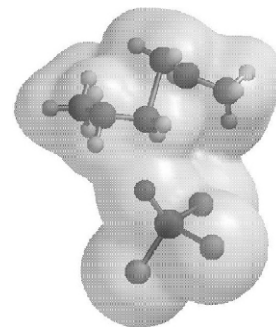


**P. Borges, R. Ramos Pinto, P. Oliveira,  
M.A.N.D.A. Lemos, F. Lemos, J.C. Védrine,  
E.G. Derouane, F. Ramôa Ribeiro**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 60

Contributions for the study of the acid transformation of hydrocarbons over zeolites

The acid-catalysed transformation of hydrocarbons has a high degree of complexity due both to the variability of the loads that are used, usually an intricate mixture of different hydrocarbons with varying reactivity, and to the fact that zeolites possess acid sites with a wide range of acid strength distribution. In this paper we intend to give a contribution to the analysis of the transformation of hydrocarbons over zeolites taking into account this latter effect. An example on the conversion of propene over ZSM-5 catalysts, with Si/Al = 15 and 24, 30 and 32%  $\text{H}^+$  exchanged by Na cations is described; in this example we show that it is possible to correlate the catalytic activity of a series of catalysts with their acid strength distribution, as measured using ammonia TPD, using Polanyi-type relationships. The use of these acidity-activity relationships allows the description of the behaviour of a set of catalysts using a single set of kinetic parameters that includes the sensitivity of the reaction to the acidity of the site and opens the way to the prediction of the activity of a catalyst based solely on the characterization of its acid site distribution.

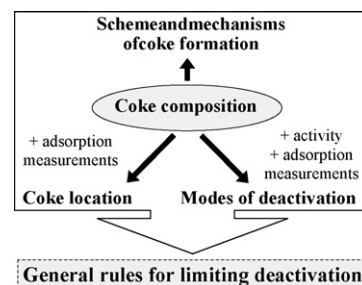


**Michel Guisnet, Luís Costa,  
Fernando Ramôa Ribeiro**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 69

Prevention of zeolite deactivation by coking

This paper presents the guidelines for preventing zeolite deactivation by coking, one of the principal phenomena responsible for the loss of activity of these catalysts in their multiple industrial applications.

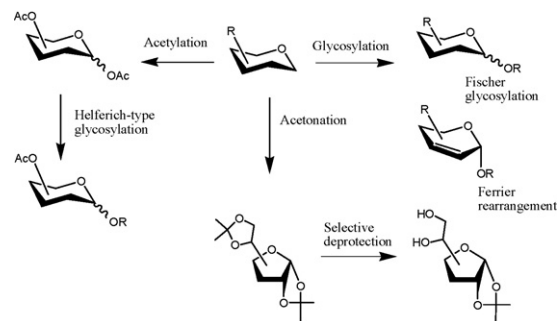


**Nuno M. Xavier, Susana D. Lucas,  
Amélia P. Rauter**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 84

Zeolites as efficient catalysts for key transformations in carbohydrate chemistry

This review covers the most significant reactions promoted by acid zeolites in carbohydrate chemistry. Key transformations such as glycosylation, sugar protection and deprotection, hydrolysis and dehydration are discussed.

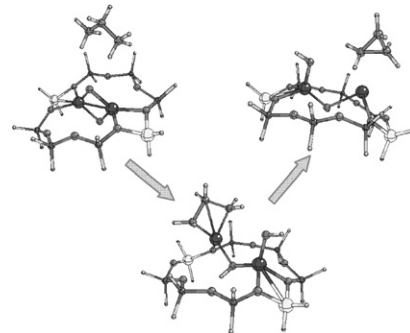


**A.V. Larin, G.M. Zhidomirov, D.N. Trubnikov,  
D.P. Vercauteren**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 90

DFT analysis of propane cyclization over binuclear Ga-clusters in mordenite

A theoretical evidence of a possibility of the cyclization of propane over Ga-form zeolites is clearly proven for the first time.

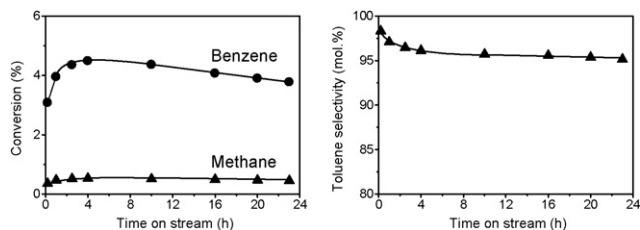


**Dmitry B. Lukyanov, Tanya Vazhnova**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 95

Selective and stable benzene alkylation with methane into toluene over PtH-MFI bifunctional catalyst

This paper demonstrates for the first time that methane reacts with benzene over bifunctional zeolite catalysts with selective and stable formation of toluene at such low temperature as 370 °C. In our view, this finding opens a new area for research into methane activation and transformation.

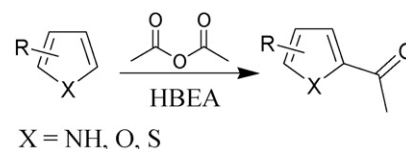


**Vasco F.D. Álvaro, Amadeu F. Brigas,  
Eric G. Derouane, João P. Lourenço,  
Bruna S. Santos**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 100

Mild liquid-phase Friedel-Crafts acylation of heteroaromatic compounds over zeolite Beta

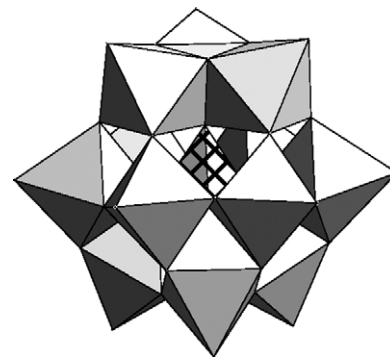
Heteroaromatic compounds, such as thiophenes, pyrroles and furans, were acylated using zeolite Beta, with and without modifications, and acetic anhydride. Amenable conditions were found to carry out these acylations in high yield, sometimes in a very short time (10 min). Indium modified catalyst have provided a way of attaining good yields in the acylation of pyrrole.



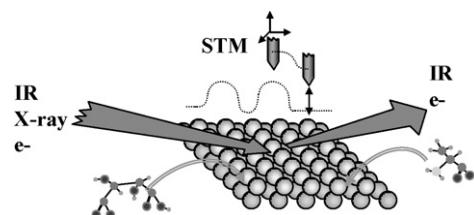
**I.V. Kozhevnikov***Journal of Molecular Catalysis A: Chemical* 305 (2009) 104

Heterogeneous acid catalysis by heteropoly acids: Approaches to catalyst deactivation

Heterogeneous acid catalysis by heteropoly acids (HPAs) has the potential of great economic rewards and green benefits. This paper discusses approaches to the problem of catalyst deactivation that could be instrumental to achieve sustainable performance of solid HPA catalysts, namely developing HPA catalysts possessing high thermal stability, modification of HPA catalysts to enhance coke combustion, inhibition of coke formation on HPA catalysts during operation, reactions in supercritical fluids and cascade reactions using multifunctional HPA catalysis.

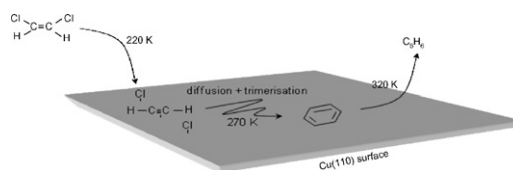
**R. Raval***Journal of Molecular Catalysis A: Chemical* 305 (2009) 112

Nanoscale insights into the creation of chiral surfaces

**S. Haq, S.C. Laroze, C. Mitchell, N. Winterton, R. Raval***Journal of Molecular Catalysis A: Chemical* 305 (2009) 117

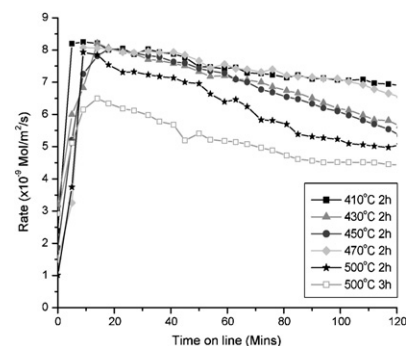
1,2-Dichloroethene on Cu(1 1 0): Adsorption, dechlorination and trimerisation reactions

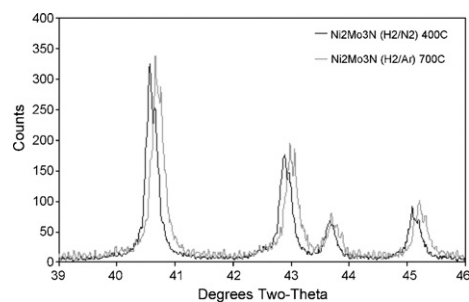
Adsorption and reactions of *cis*-1,2-dichloroethene on Cu(1 1 0) can be described in terms of three main regimes: I (<150 K) intact molecular adsorption; II (155–280 K) desorption/dechlorination; and finally, III (>280–450 K) trimerisation of the acetylene intermediate at the surface to form benzene which desorbs above 350 K. Although the related positions of the Cl atoms force different adsorption geometries for *cis*- and *trans*-1,2-dichloroethene, the behaviour of the two compounds is similar. No isomerisation between the *cis* and *trans* isomers was seen.

**Christopher Jones, Kieran J. Cole, Stuart H. Taylor, Mandy J. Crudace, Graham J. Hutchings***Journal of Molecular Catalysis A: Chemical* 305 (2009) 121

Copper manganese oxide catalysts for ambient temperature carbon monoxide oxidation: Effect of calcination on activity

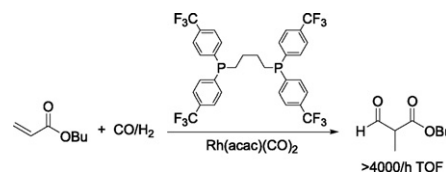
Hopcalite  $\text{CuMnO}_x$ , prepared by coprecipitation from an aqueous solution of copper and manganese nitrates, is very active for CO oxidation at ambient temperature. The activity is principally affected by two features, namely the surface area and the phase composition. Both of these features are controlled by the temperature used for the calcination.



**J.S.J. Hargreaves, D. Mckay***Journal of Molecular Catalysis A: Chemical* 305 (2009) 125A comparison of the reactivity of lattice nitrogen in  $\text{Co}_3\text{Mo}_3\text{N}$  and  $\text{Ni}_2\text{Mo}_3\text{N}$  catalysts**Ourida Saidi, Shifang Liu, Jianliang Xiao***Journal of Molecular Catalysis A: Chemical* 305 (2009) 130

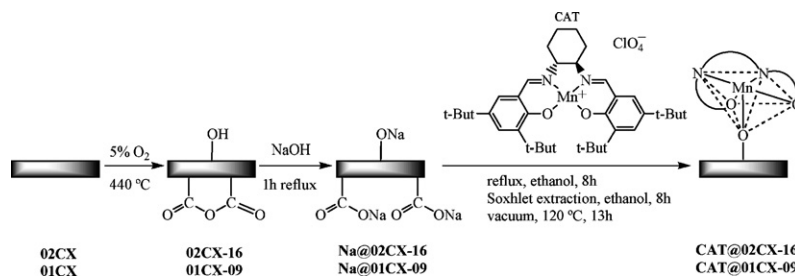
Effects of ligands on the rhodium-catalyzed hydroformylation of acrylate

Electron-deficient diphosphine is shown to enhance the rate of rhodium-catalyzed hydroformylation of acrylate, whilst the electron-rich analogue affords the opposite.

**Frederico Maia, Nagendranath Mahata, Bruno Jarrais, Ana R. Silva, Manuel Fernando R. Pereira, Cristina Freire, José Luís Figueiredo***Journal of Molecular Catalysis A: Chemical* 305 (2009) 135

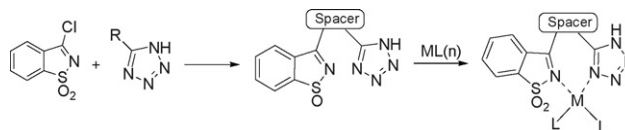
Jacobsen catalyst anchored onto modified carbon xerogel as enantioselective heterogeneous catalyst for alkene epoxidation

Anchoring of the Jacobsen catalyst (CAT) onto carbon xerogels (CX)

**Luís M.T. Frija, R. Fausto, Rui M.S. Loureiro, M. Lurdes S. Cristiano***Journal of Molecular Catalysis A: Chemical* 305 (2009) 142

Synthesis and structure of novel benzisothiazole-tetrazolyl derivatives for potential application as nitrogen ligands

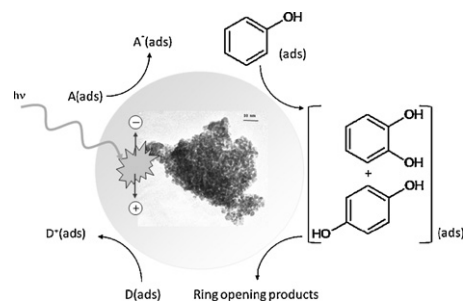
Novel benzisothiazole-tetrazolyl derivatives, differing on the spacer-group used for linkage of the two heterocycles, were devised. The application of these compounds as nitrogen ligands for coordination with transition metals was also explored.



**Cláudia Gomes Silva, Joaquim Luís Faria**
*Journal of Molecular Catalysis A: Chemical* 305 (2009) 147

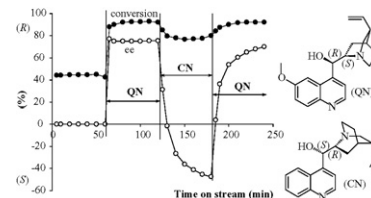
Effect of key operational parameters on the photocatalytic oxidation of phenol by nanocrystalline sol-gel TiO<sub>2</sub> under UV irradiation

Nanocrystalline sol-gel TiO<sub>2</sub> catalysts are synthesized for use in the photocatalytic oxidation of phenol under UV irradiation. Pure anatase nanocrystallites (8.5 nm) are very efficient photocatalysts. However as the rate of oxidation increases with the intensity of incident light, desorption induced by light absorption also increases, limiting the overall efficiency of the process.

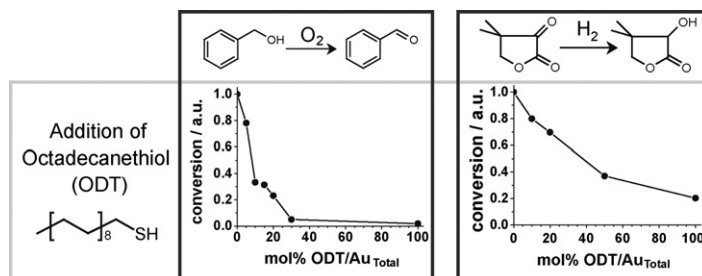

**György Szöllösi, Szabolcs Cserényi, Katalin Balázsik, Ferenc Fülöp, Mihály Bartók**
*Journal of Molecular Catalysis A: Chemical* 305 (2009) 155

New data in the enantioselective hydrogenation of ethyl pyruvate on Pt-cinchona chiral catalyst using continuous-flow fixed-bed reactor system: The origin of rate enhancement

New data were obtained in a continuous-flow fixed-bed reactor, supporting the “ligand acceleration” origin of the rate enhancement in the enantioselective heterogeneous hydrogenation of ethyl pyruvate.

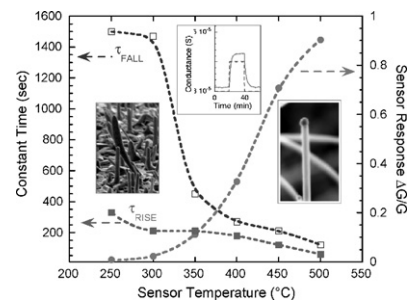

**Peter Haider, Atsushi Urakawa, Erik Schmidt, Alfons Baiker**
*Journal of Molecular Catalysis A: Chemical* 305 (2009) 161

Selective blocking of active sites on supported gold catalysts by adsorbed thiols and its effect on the catalytic behavior: A combined experimental and theoretical study


**Elisabetta Comini, Guido Faglia, Matteo Ferroni, Andrea Ponzoni, Alberto Vomiero, Giorgio Sberveglieri**
*Journal of Molecular Catalysis A: Chemical* 305 (2009) 170

Metal oxide nanowires: Preparation and application in gas sensing

Quasi one-dimensional nanowires of metal oxides are promising for the development of nano-devices. Sn, In, and Zn oxides were produced in form of single-crystalline nanowires through condensation from vapor phase. Furthermore longitudinal and radial heterostructures have been prepared. Preparation, microstructural, morphological and electrical characterizations of nanowires are presented and the peculiarities of these innovative structures are highlighted.



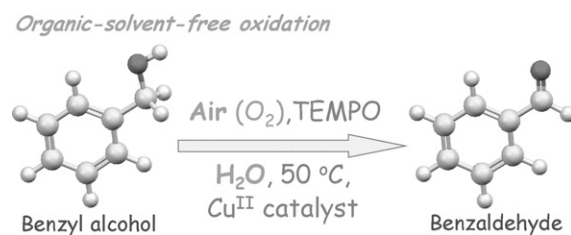


**Paweł J. Figiel, Alexander M. Kirillov,  
Yauhen Yu. Karabach, Maximilian N. Kopylovich,  
Armando J.L. Pombeiro**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 178

Mild aerobic oxidation of benzyl alcohols to benzaldehydes in water catalyzed by aqua-soluble multicopper(II) triethanolaminate compounds

Aqua-soluble multicopper(II) compounds are shown to act as efficient catalysts for the mild and selective oxidation of benzyl alcohols to benzaldehydes (up to 99% yield), which is mediated by TEMPO radical and does not require the conventional use of any organic solvent or an ionic liquid, proceeding in sole water at 50 °C under atmospheric pressure of air as oxidant.



**J.J. Birtill**

*Journal of Molecular Catalysis A: Chemical* 305 (2009) 183

Some experiences in industrial catalysis

Some case histories are presented to illustrate aspects of industrial applied catalysis research, including the interrelation of scientific and commercial factors in techno-commercial evaluation, and the importance of realistic target setting.

