

## Contents

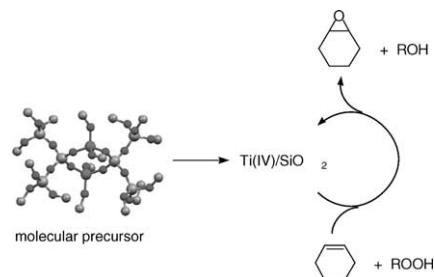
### Articles

**Richard L. Brutchey, Benjamin V. Mork, Donald J. Sirbulu, Peidong Yang, T. Don Tilley**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 1

A dimeric molecular precursor  $[(t\text{BuO})_2\text{Ti}\{\mu\text{-O}_2\text{Si}[\text{OSi}(\text{O}^t\text{Bu})_3]_2\}]_2$  to Ti(IV)/SiO<sub>2</sub> catalysts for selective cyclohexene epoxidation

Active and selective Ti(IV)/SiO<sub>2</sub> catalysts for cyclohexene epoxidation were prepared by the thermolytic molecular precursor route with a dimeric molecular precursor  $[(t\text{BuO})_2\text{Ti}\{\mu\text{-O}_2\text{Si}[\text{OSi}(\text{O}^t\text{Bu})_3]_2\}]_2$ . The catalytic effects of using a molecular dimeric Ti(IV) source was examined as compared to catalysts prepared using monomeric Ti(IV) sources.

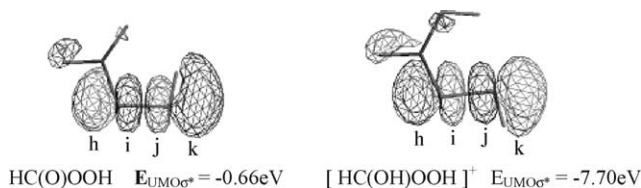


**Hongchang Shi, Zhiguo Zhang, Yilui Wang**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 13

Mechanism on epoxidation of alkenes by peracids: A protonation-promoted pathway and its quantum chemical elucidation

The orbital energies  $E_{\text{UMO}\sigma^*}$  of the UMOs in which  $\sigma^*$  orbital of peroxy bond of protonated peracids are 5–7 eV lower than those of neutral peracids, which greatly increases the epoxidation reactivity of peracids.

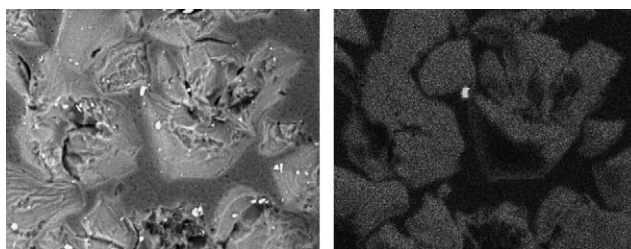


**C. Burato, P. Centomo, G. Pace, M. Favaro, L. Prati, B. Corain**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 26

Generation of size-controlled palladium(0) and gold(0) nanoclusters inside the nanoporous domains of gel-type functional resins  
Part II: Prospects for oxidation catalysis in the liquid phase

Distribution of gold through a section of a MTEMA-DMAA 4–6 particle.

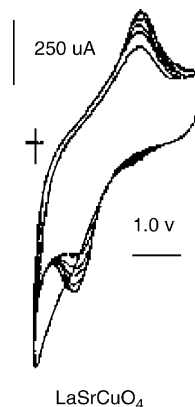


**Junjiang Zhu, Zhen Zhao, Dehai Xiao, Jing Li, Xiangguang Yang, Yue Wu**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 35

Study of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  ( $x = 0.0, 0.5, 1.0$ ) catalysts for NO + CO reaction from the measurements of  $\text{O}_2$ -TPD,  $\text{H}_2$ -TPR and cyclic voltammetry

With the link of oxygen vacancy, CV was introduced and has obtained great success in explaining reaction in heterogeneous catalysis.

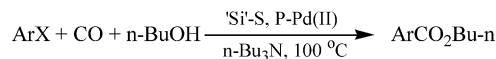
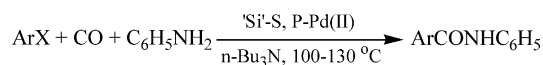


**Mingzhong Cai, Hong Zhao, Yixiang Huang**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 41

Carbonylation of aryl halides catalyzed by a silica-supported sulfur and phosphine mixed bidentate palladium complex

The silica-supported sulfur and phosphine mixed bidentate palladium complex ('Si'-S, P-Pd(II)) is an efficient catalyst for Heck carbonylation of aryl halides with aniline or *n*-butyl alcohol under atmospheric pressure of carbon monoxide and can be recovered and reused without loss of activity.



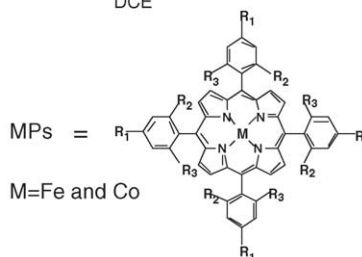
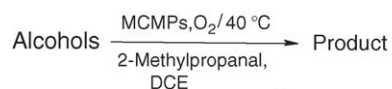
X = I, Br

**Rajan Naik, Padmakar Joshi, Rajesh K. Deshpande**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 46

Immobilization of metalloporphyrins on polystyrene: Efficient catalysts for aerobic oxidation of alcohols

Metalloporphyrins of iron and cobalt have been successfully immobilized for the first time using polystyrene matrix and are used as efficient catalysts for aerobic oxidation of alcohols.

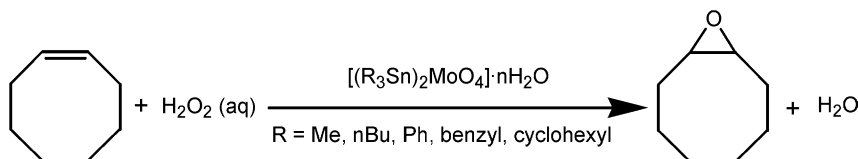


**Marta Abrantes, Anabela A. Valente, Isabel S. Gonçalves, Martyn Pillinger, Carlos C. Romão**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 51

Organotin-oxomolybdate coordination polymers as catalysts for the epoxidation of cyclooctene

A series of organotin-oxomolybdate coordination polymers were tested as catalysts for the liquid-phase epoxidation of cyclooctene with aqueous hydrogen peroxide at 35°C and atmospheric pressure. Water, acetonitrile and dichloromethane were examined as additional co-solvents for the reaction. The catalytic results vary considerably according to the nature of the tin-bound *R* group and the co-solvent.

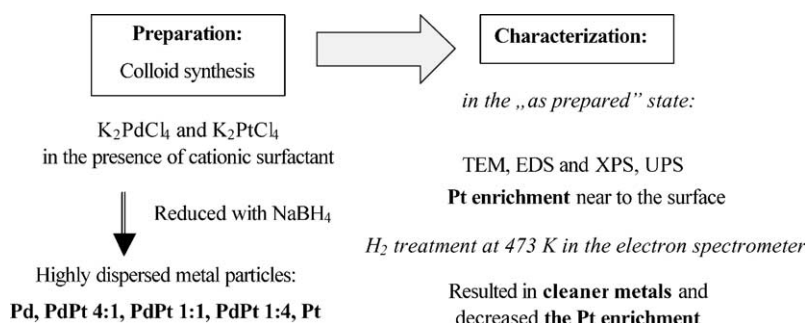


**B. Veisz, L. Tóth, D. Teschner, Z. Paál,  
N. Györfly, U. Wild, R. Schlögl**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 56

Palladium-platinum powder catalysts manufactured by colloid synthesis

I. Preparation and characterization

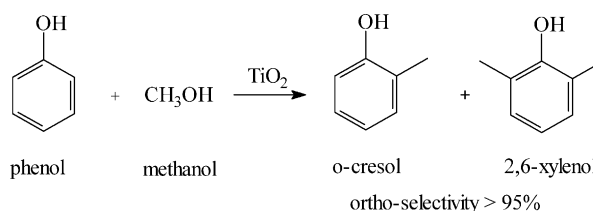


**Aditi R. Gandhe, Julio B. Fernandes,  
Salil Varma, N.M. Gupta**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 63

$TiO_2$ : As a versatile catalyst for the ortho-selective methylation of phenol

Mesoporous  $TiO_2$  catalysts synthesized from urea-oxalate precursors of  $TiCl_3$  exhibit near 100% ortho-selectivity in the methylation of phenol.

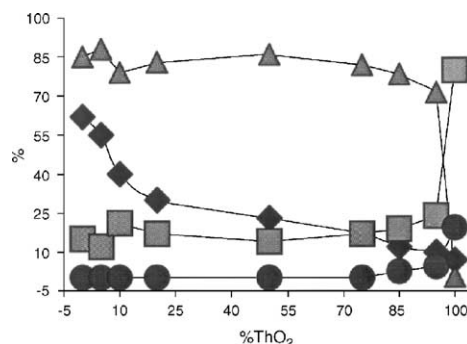


**Hossein A. Dabbagh, Mohammadsadegh  
Yalfani, Burtron H. Davis**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 72

An XRD and Fourier-transformed infrared spectroscopy investigation of single and mixed  $\gamma$ -alumina and thorium oxide

Catalytic activity and selectivity data show that mixed thoria-alumina catalysts resemble alumina up to 90% or greater thoria content.

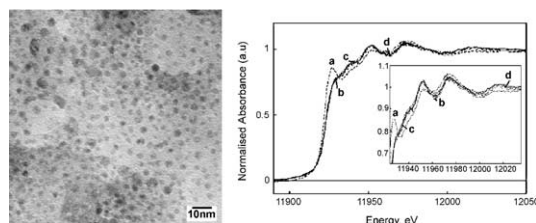


**Deepak B Akolekar, Suresh K Bhargava,  
Garry Foran, Masashi Takahashi**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 78

Studies on gold nanoparticles supported on iron, cobalt, manganese, and cerium oxide catalytic materials

Gold nanoparticles containing iron, cobalt, manganese and cerium materials were prepared and characterized by the ICP-MS, TGA, TEM, XRD, BET, Mössbauer and XAS techniques. Au  $L_3$  edge X-ray absorption spectroscopic measurements were carried out over a series of transition and rare earth materials containing gold nanoparticles. XAFS and in-situ high temperature XRD techniques were used to investigate the influence of the high temperature treatment on gold nanoparticles inside the metal oxide materials.

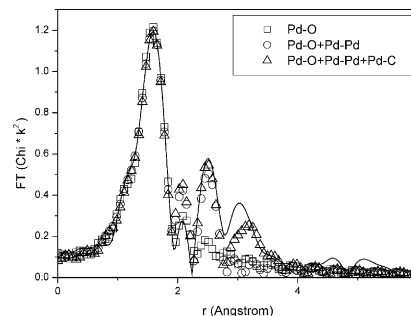


**Shawn D. Lin, Yin-Hou Hsu, Po-Hau Jen, Jyh-Fu Lee**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 88

Probing Pd–carbon interaction in Pd/C catalysts by EXAFS

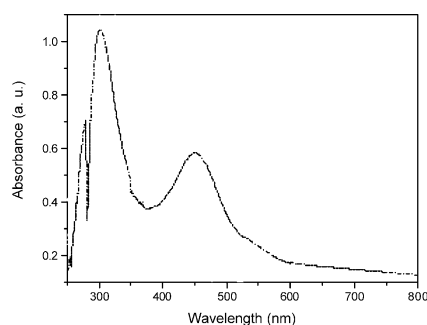
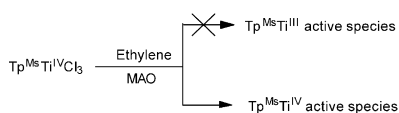
A Pd–C shell at ca. 3.6 Å can be included in the EXAFS fitting to the Pd/C catalyst prepared by PdCl<sub>2</sub> or Pd(NO<sub>3</sub>)<sub>2</sub> impregnation. The model of precursor anchoring by surface oxygen groups is not supported by EXAFS. This Pd–C interaction was originally proposed [1] for Pd(NH<sub>3</sub>)<sub>4</sub>Cl<sub>2</sub>/C. It indicates the presence of a similar Pd–C interaction in the Pd/C catalysts from cationic, anionic, and neutral Pd precursors.



**Marcelo P. Gil, J.H.Z. dos Santos, O.L. Casagrande, Lílían M.T. Simplicio, Zênis N. da Rocha**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 96

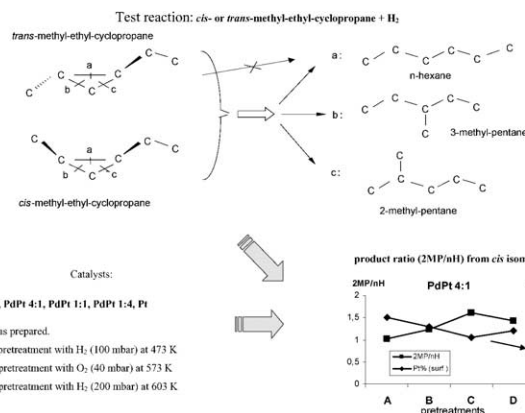
Spectroscopic and voltametric studies in titanium tris(pyrazolyl)borate catalysts



**N. Györfy, L. Tóth, M. Bartók, J. Ocskó, U. Wild, R. Schlögl, D. Teschner, Z. Paál**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 102

Palladium-platinum powder catalysts manufactured by colloid synthesis  
II. Characterization and Catalytic tests after oxidizing and reducing treatment

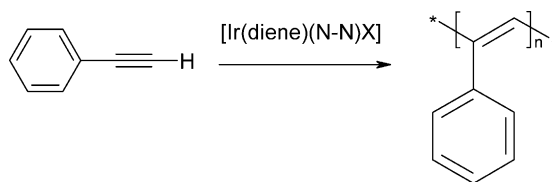


**Serena Filipuzzi, Erica Farnetti**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 111

Organoiridium compounds with substituted phenantrolines as alkynes polymerization catalysts

The iridium derivatives [Ir(diene)(N–N)X] (diene = 1,5-cyclooctadiene, 1,5-hexadiene; N–N = 1,10-phenantroline and substituted derivatives; X = Cl, Br, I) catalyze the polymerization of phenylacetylene to the corresponding trans-polyene. The reaction is highly stereoselective with formation of 100% *trans*-polyphenylacetylene. A pronounced effect of the donor properties of the ligands on the catalytic reaction was observed. Spectroscopic studies provided useful indications as regards the formation of the polymerization initiator.

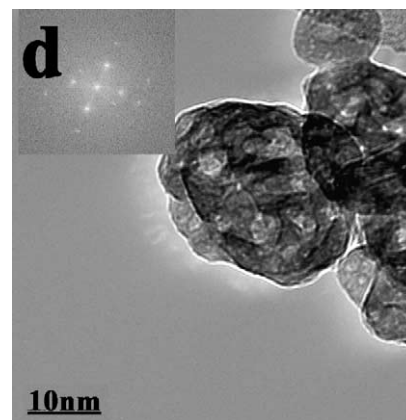


**Tianyou Peng, De Zhao, Haibo Song, Chunhua Yan**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 119

Preparation of lanthana-doped titania nanoparticles with anatase mesoporous walls and high photocatalytic activity

Lanthana-doped mesoporous  $\text{TiO}_2$  nanoparticles with high specific surface area and anatase wall was synthesized via hydrothermal process. The obtained doped  $\text{TiO}_2$  nanoparticles have mean diameter of 20 nm with mean pore size of 2.2 nm. The specific surface area of the samples after calcination at  $500^\circ\text{C}$  still have  $243\text{m}^2/\text{g}$ . The doped  $\text{TiO}_2$  nanoparticles show better activities than P25 on the oxidation of rhodamine B.

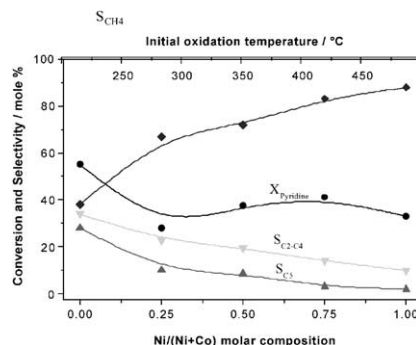


**Sergio L. González-Cortés, Tian-Cun Xiao, Pedro M.F.J. Costa, Serbia M.A. Rodulfo-Baechler, Malcolm L.H. Green**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 127

Relevance of the  $\text{Co}_{1-x}\text{Ni}_x\text{WO}_4$  wolframite-type mixed oxide compositions on the synthesis and catalytic properties of W-based carbides

A series of wolframite-type oxides ( $\text{Co}_{1-x}\text{Ni}_x\text{WO}_4$ ) with various compositions was prepared by urea-matrix combustion method and subsequently carburized using temperature-programmed reaction. The carbide catalysts were active for the pyridine HDN reaction. The HDN active phase presents in  $\text{CoWC}_x$  is different than that presents in the Ni-containing catalysts.

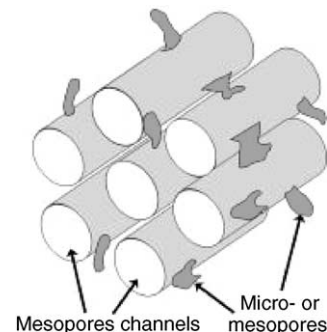


**C.G. Sonwane, Peter J. Ludovice**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 135

A note on micro- and mesopores in the walls of SBA-15 and hysteresis of adsorption isotherms

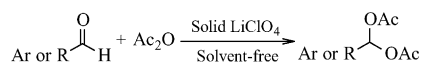
Unlike MCM-41, SBA-15 consists of randomly arranged micro- and mesopores in the walls. The presence of hysteresis in adsorption isotherm of condensable gases in SBA-15 or MCM-41 depends on the properties of adsorbate determined by pore diameter and temperature. The bulges/neck, U-shaped pores/sinuosity and micropores present in SBA-15 do not have any influence on the existence of hysteresis.



**Azim Ziyaei, Najmedin Azizi, Mohammad R. Saidi**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 138

Chemoselective and convenient preparation of 1,1-diacetates from aldehydes, mediated by solid lithium perchlorate under solvent-free conditions

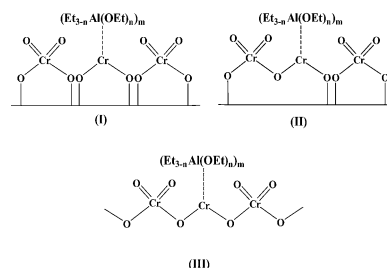


**Boping Liu, Pavel Šindelář, Yuwei Fang,  
Kouichi Hasebe, Minoru Terano**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 142

Correlation of oxidation states of surface chromium species with ethylene polymerization activity for Phillips  $\text{CrO}_x/\text{SiO}_2$  catalysts modified by Al-alkyl cocatalyst

Correlation of oxidation states of surface Cr species on TEA-modified Phillips catalysts with their ethylene polymerization activity in terms of catalyst calcination temperature and Al/Cr molar ratio suggested that the real active Cr precursor might be a  $\text{Cr}^{2+}\cdot 2\text{Cr}^{6+}$  cluster (Scheme 1). Based on this plausible cluster model, the active sites concentration is estimated to be around 14.4–24.9 (mol% Cr) for the TEA-modified Phillips catalysts.

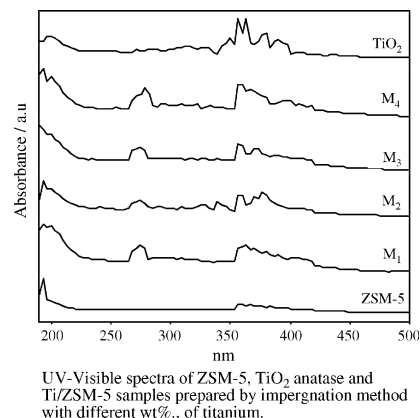


**R.M. Mohamed, A.A. Ismail, I. Othman,  
I.A. Ibrahim**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 151

Preparation of  $\text{TiO}_2$ -ZSM-5 zeolite for photodegradation of EDTA

Doping of  $\text{TiO}_2$  into ZSM-5 zeolite has been achieved by impregnation and solid–solid interaction methods. The incorporation of titanium into framework of ZSM-5 using impregnation method is higher than that of solid–solid interaction method. The photodegradation of EDTA by impregnation method is much better than that of solid–solid interaction method.

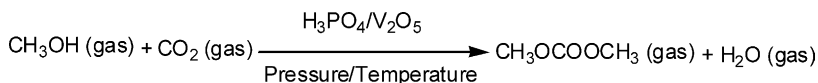


**X.L. Wu, M. Xiao, Y.Z. Meng, Y.X. Lu**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 158

Direct synthesis of dimethyl carbonate on  $\text{H}_3\text{PO}_4$  modified  $\text{V}_2\text{O}_5$

The catalytic properties and mechanism of  $\text{H}_3\text{PO}_4$  modified  $\text{V}_2\text{O}_5$  catalysts for the direct synthesis of dimethyl carbonate (DMC) from  $\text{CO}_2$  and  $\text{CH}_3\text{OH}$  were investigated by means of DRIFT and XRD technologies, and the experimental results showed that the modified  $\text{V}_2\text{O}_5$  catalysts were effective for the direct and selective synthesis of DMC from  $\text{CO}_2$  and  $\text{CH}_3\text{OH}$ . The crystal phase of  $\text{V}_2\text{O}_5$  influenced greatly on the reaction yield and selectivity of DMC.

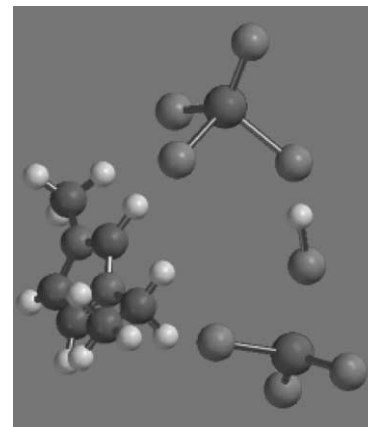


**Ernesto J. Angueira, Mark G. White**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 163

Ionic liquid structure effect upon reactivity of toluene carbonylation: 1. Organic cation structure

Modeling of ionic liquids derived from  $\text{AlCl}_3/1\text{-R-3-Me-imidazolium}$  chloride ( $\text{R} = \text{ethyl, } n\text{-butyl, benzyl, } n\text{-hexyl, } n\text{-octyl, } n\text{-dodecyl}$ ) by semi-empirical methods shed light on the observed activity patterns in toluene carbonylation as the R-group was changed.

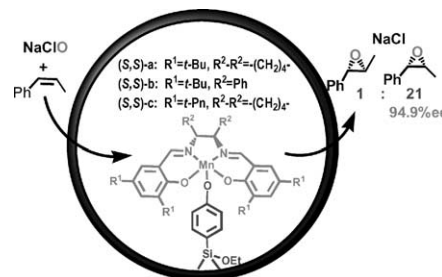


Huidong Zhang, Song Xiang, Jianliang Xiao, Can Li

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 175

Heterogeneous enantioselective epoxidation catalyzed by Mn(salen) complexes grafted onto mesoporous materials by phenoxy group

Three chiral Mn(salen) complexes immobilized into various mesoporous materials via phenoxy group by a simplified method show remarkably higher ee values for asymmetric epoxidation of  $\alpha$ -methylstyrene (79.7 versus 26.4%) and *cis*- $\beta$ -methylstyrene (94.9 versus 25.3%) than the homogeneous catalysts. The heterogeneous catalysts also obviously alter the *cis/trans* ratio of epoxide (homogeneous 0.38 versus heterogeneous 21).

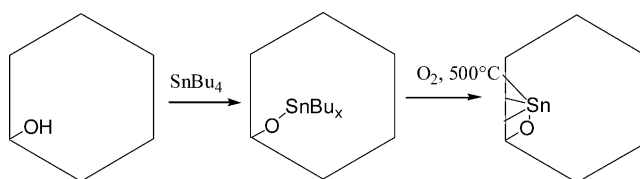


Xuxu Wang, Haibing Xu, Xianzhi Fu, Ping Liu, Frédéric Lefebvre, Jean-Marie Basset

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 185

Characterization and catalytic properties of tin-containing mesoporous silicas prepared by different methods

Well-characterized tin containing MCM-41 are prepared by reacting hydroxyl groups with tetrabutyl tin and further calcinations.

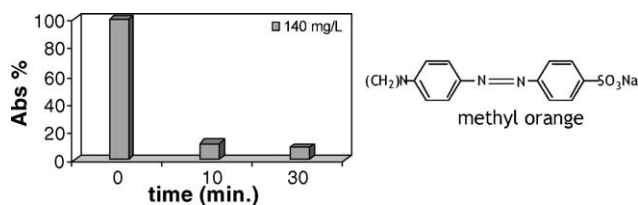


Arménio C. Serra, Cristina Docal, A.M.d'A. Rocha Gonsalves

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 192

Efficient azo dye degradation by hydrogen peroxide oxidation with metalloporphyrins as catalysts

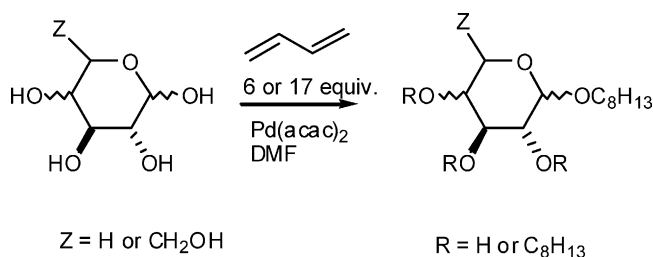
An efficient azo dye degradation system using diluted hydrogen peroxide solutions as oxidant and metalloporphyrins as catalysts is disclosed.



Alla Bessmertnykh, Françoise Hénin, Jacques Muzart

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 199

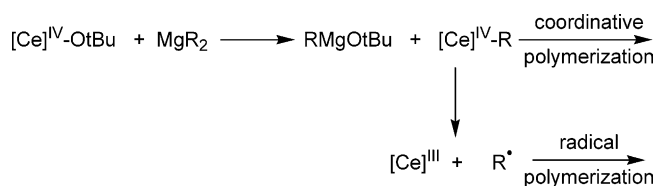
Palladium-catalysed telomerization of butadiene with aldoses: A convenient route to non-ionic surfactants based on controlled reactions



**Yann Sarazin, Thomas Chenal,  
André Mortreux, Hervé Vezin,  
Jean-François Carpentier**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 207

Binary cerium(IV) *tert*-butoxides-dialkylmagnesium systems: Radical versus coordinative polymerization of styrene



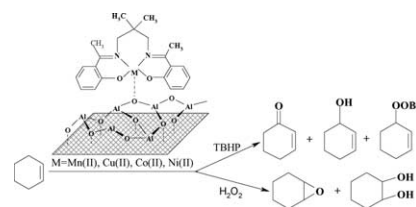
**Masoud Salavati-Niasari, Parinaz Salemi,  
Fateme Davar**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 215

Oxidation of cyclohexene with *tert*-butylhydroperoxide and hydrogen peroxide catalyzed by Cu(II), Ni(II), Co(II) and Mn(II) complexes of *N,N'*-bis-( $\alpha$ -methylsalicylidene)-2,2-dimethylpropane-1,3-diamine, supported on alumina

New square-planar manganese(II), copper(II), nickel(II) and cobalt(II) complexes of a tetradentate Schiff-base ligand "*N,N'*-bis-( $\alpha$ -methylsalicylidene)-2,2-dimethylpropane-1,3-diamine,  $\text{H}_2[\text{Me}_2\text{salpnMe}_2]$ " have been prepared and characterized by elemental analyses, IR, UV-vis, conductometric and magnetic measurements. The results suggest that the symmetrical Schiff-base is a bivalent anion with tetradentate ONNO donors derived from the phenolic oxygen and azomethine nitrogen. The formulae was found to be  $[\text{M}(\text{Me}_2\text{salpnMe}_2)]$  for the 1:1 non-electrolytic complexes. Alumina-supported metal complexes (ASMC);  $[\text{M}(\text{Me}_2\text{salpnMe}_2)/\text{Al}_2\text{O}_3]$ ; catalyze the oxidation of cyclohexene with *tert*-butylhydroperoxide (TBHP) and hydrogen peroxide.

Manganese(II) complex supported on alumina " $[\text{Mn}(\text{Me}_2\text{salpnMe}_2)/\text{Al}_2\text{O}_3]$ " shows significantly higher catalytic activity than other catalysts.

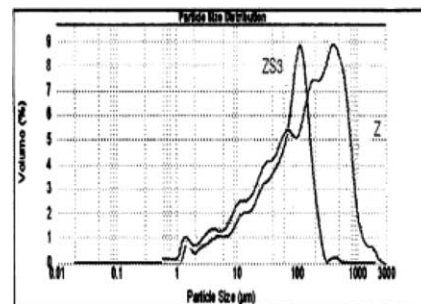


**Nikunj Bhatt, Anjali Patel**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 223

Esterification of 1° and 2° alcohol using an ecofriendly solid acid catalyst comprising 12-tungstosilicic acid and hydrous zirconia

A series of ecofriendly solid acid catalysts was synthesised by supporting 12-tungstosilicic acid onto hydrous zirconia. The support and resulting catalyst was characterized by various spectral, thermal and physicochemical techniques. Their catalytic properties were evaluated for the esterification of *n*-butanol, iso-butanol, 2-butanol and cyclohexanol with different acid.

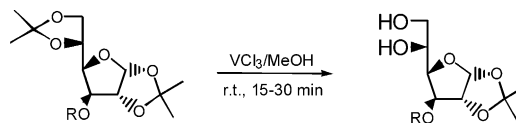


**Gowravaram Sabitha, G.S.Kiran Kumar Reddy,  
K. Bhaskar Reddy, N. Mallikarjuna Reddy,  
J.S. Yadav**

*Journal of Molecular Catalysis A: Chemical* 238  
(2005) 229

Vanadium(III) chloride: A mild and efficient catalyst for the chemoselective deprotection of acetonides

Acetonides are selectively cleaved at room temperature by a catalytic amount of  $\text{VCl}_3$  in methanol to furnish the corresponding diols under mild conditions. Other hydroxyl protecting groups such as TBDMS, TBDS, AC, THP, Bn, prenyl, allyl present in the substrate were intact under the reaction conditions.



R = H, Bn, TBDMS, THP, Ac, prenyl, Allyl

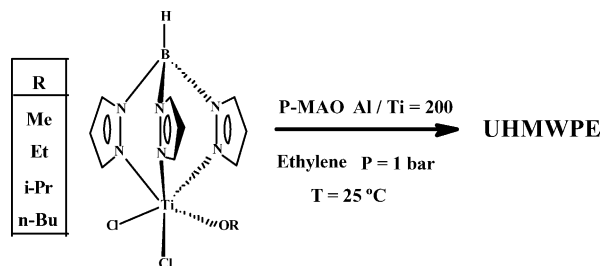


**Arquimedes Karam, Emilio Casas, Edgar Catari, Sara Pekerar, Alberto Albornoz, Bernardo Méndez**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 233

Effect of the alkoxyl ligands on ethylene polymerization by  $\text{TpTiCl}_2(\text{OR})$  complexes

The  $\text{TpTiCl}_2(\text{OR})$  complexes activated with very low concentration of MAO showed very high activity in the ethylene polymerization. The alkoxyl ligands strongly affect the catalytic and the molecular weights of the polymers, prevailing the steric effect over the electronic effect. The resulting polymers can be classified as ultra-high molecular weight polyethylenes with basically linear structure.



**Baohua Yue, Renxian Zhou, Yuejuan Wang, Xiaoming Zheng**

*Journal of Molecular Catalysis A: Chemical* 238 (2005) 241

Study of the methane combustion and TPR/TPO properties of  $\text{Pd/Ce-Zr-M/Al}_2\text{O}_3$  catalysts with  $\text{M} = \text{Mg, Ca, Sr, Ba}$

The effects of alkaline earths (Mg, Ca, Sr and Ba) addition to  $\text{Pd/Ce-Zr/Al}_2\text{O}_3$  catalyst on methane combustion behavior have been investigated. The addition of Ca to  $\text{Pd/Ce-Zr/Al}_2\text{O}_3$  inhibits the site growth and decomposition of  $\text{PdO}$  particles and improves the reduction-reoxidation properties of the active  $\text{PdO}$  species, which increases the catalytic activity and thermal stability of the  $\text{Pd/Ce-Zr/Al}_2\text{O}_3$  catalyst.

