



## Contents

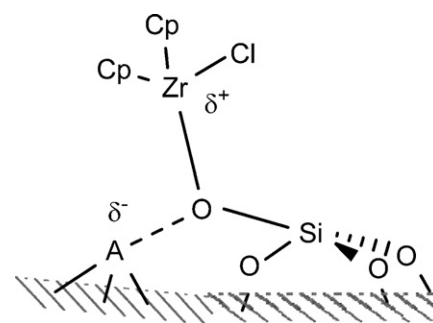
### Articles

**João M. Campos, João Paulo Lourenço,  
Auguste Fernandes, Ana Maria Rego,  
M. Rosário Ribeiro**

*Journal of Molecular Catalysis A: Chemical 310 (2009) 1*

Mesoporous Ga-MCM-41 as support for metallocene catalysts: Acidity–activity relationship

A model is presented for the interactions between  $\text{Cp}_2\text{ZrCl}_2$  and the acid sites present in Ga-MCM-41 materials, establishing an interpretation of the catalytic behaviour based on an acidity–activity relationship.

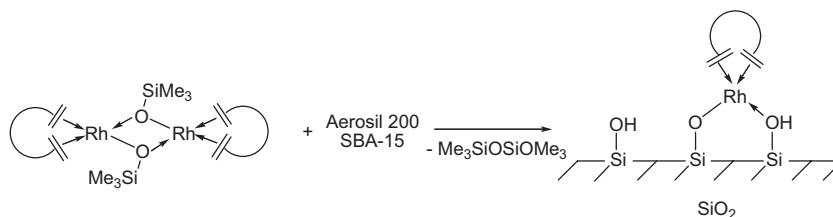


**Bogdan Marciniak, Karol Szubert,  
Ryszard Fiedorow, Ireneusz Kownacki,  
Marek J. Potrzebowski, Michał Dutkiewicz,  
Adrian Franczyk**

*Journal of Molecular Catalysis A: Chemical 310 (2009) 9*

Catalysis of hydrosilylation by well-defined rhodium siloxide complexes immobilized on silica

Well-defined rhodium siloxide surface complexes prepared directly from molecular precursors [ $\{\text{Rh}(\mu\text{-OSiMe}_3)(\text{diene})_2\}$ ] characterized by solid-state MAS NMR spectroscopy appear to be highly effective catalysts for hydrosilylation of olefins.

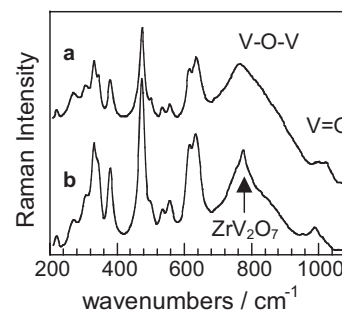


**Delia Gazzoli, Sergio De Rossi, Giovanni Ferraris,  
Giorgio Mattei, Roberto Spinicci, Mario Valigi**

*Journal of Molecular Catalysis A: Chemical 310 (2009) 17*

Bulk and surface structures of  $\text{V}_2\text{O}_5/\text{ZrO}_2$  catalysts for *n*-butane oxidative dehydrogenation

The catalysts mainly contain polymeric vanadium structures (a), partly interacting with the support surface (b). The exposed polymeric V–O–V structures are associated with the ODH reaction activity, whereas Zr–O–V sites favour alkane combustion.



**Puttaswamy, Anu Sukhdev, J.P. Shubha***Journal of Molecular Catalysis A: Chemical* 310 (2009) 24

Kinetics and reactivities of ruthenium(III)- and osmium(VIII)-catalyzed oxidation of ornidazole with chloramine-T in acid and alkaline media: A mechanistic approach

Ru(III)- and Os(VIII)-catalyzed kinetics of oxidation of ornidazole with chloramine-T in HCl and NaOH media exhibit different kinetic patterns. Under comparable experimental conditions, in Ru(III)-catalyzed oxidation the rate law is The proposed mechanisms and the derived rate laws are substantiated by all the experimental facts.

$$-d[\text{CAT}] / dt = \frac{K_1 K_2 K_3 k_4 [\text{CAT}]_t [\text{ornidazole}] [\text{Ru(III)}]}{[\text{H}^+] + K_1 + K_1 K_2 [\text{Ru(III)}] + K_1 K_2 K_3 [\text{ornidazole}] [\text{Ru(III)}]}$$

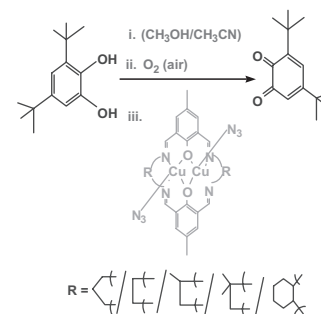
and for Os(VIII) catalyzed reaction it takes the form

$$-d[\text{CAT}] / dt = \frac{K_6 K_7 k_8 [\text{CAT}]_t [\text{ornidazole}] [\text{OH}^-] [\text{Os(VIII)}]}{[\text{ArSO}_2\text{NH}_2] + K_6 [\text{OH}^-] + K_6 K_7 [\text{ornidazole}] [\text{OH}^-]}$$

**Kazi Sabnam Banu, Tanmay Chattopadhyay, Arpita Banerjee, Santanu Bhattacharya, Ennio Zangrando, Debasis Das***Journal of Molecular Catalysis A: Chemical* 310 (2009) 34

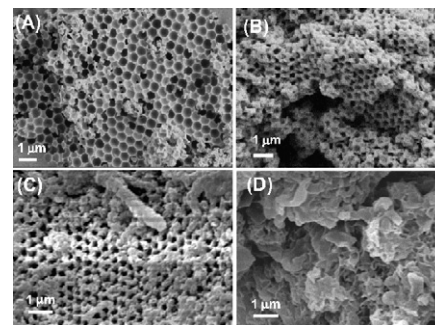
Catechol oxidase activity of dinuclear copper(II) complexes of macrocyclic ligands has been investigated to understand the role of chelate ring size, steric, electronic and that of solvent.

Catechol oxidase activity of dinuclear copper(II) complexes of macrocyclic ligands has been investigated to understand the role of chelate ring size, steric, electronic and that of solvent.

**Matilte Halma, Kelly Aparecida Dias de Freitas Castro, Vanessa Prévot, Claude Forano, Fernando Wypych, Shirley Nakagaki***Journal of Molecular Catalysis A: Chemical* 310 (2009) 42

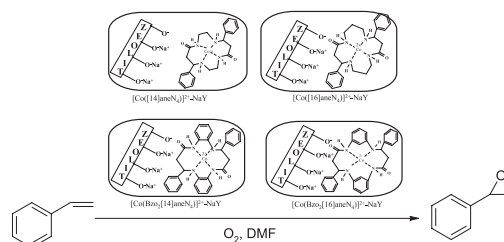
Immobilization of anionic iron(III) porphyrins into ordered macroporous layered double hydroxides and investigation of catalytic activity in oxidation reactions

The anionic iron(III) porphyrins were immobilized into three-dimensionally macroporous layered double hydroxide (3DM-LDH), using the direct reconstruction of 3DM-LDH from macroporous mixed oxides MOX or the anionic exchange on DDS intercalated 3DM-LDH. The obtained materials were investigated as catalysts for oxidation reactions and presented good results for oxidation of terminal positions of linear alkanes.

**Masoud Salavati-Niasari***Journal of Molecular Catalysis A: Chemical* 310 (2009) 51

Synthesis, characterization of cobalt(II) complex nanoparticles encapsulated within nanoreactors of zeolite-Y and their catalytic activities

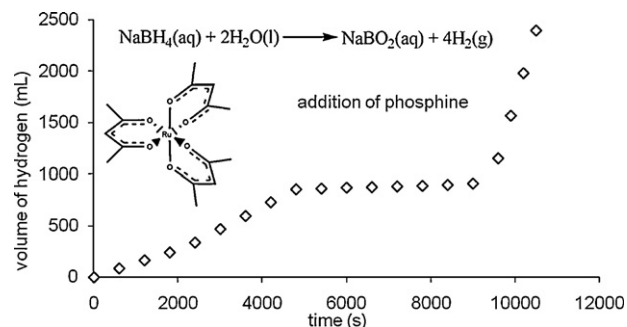
Cobalt(II) complex nanoparticles of [14]aneN<sub>4</sub>: 1,5,8,12-tetraaza-2,9-dioxo-4,11-diphenylcyclotetradecane; [16]aneN<sub>4</sub>: 1,5,9,13-tetraaza-2,10-dioxo-4,12-diphenylcyclohexadecane; Bzo<sub>2</sub>[14]aneN<sub>4</sub>: dibenzo-1,5,8,12-tetraaza-2,9-dioxo-4,11-diphenylcyclotetradecane and Bzo<sub>2</sub>[16]aneN<sub>4</sub>: dibenzo-1,5,9,13-tetraaza-2,10-dioxo-4,12-diphenylcyclohexadecane have been encapsulated in the nanopores of zeolite-Y. The new complex nanoparticles entrapped in the nanoreactor of zeolite-Y were characterized by deferent techniques. These complexes (neat and encapsulated) were used for epoxidation of styrene with O<sub>2</sub> as oxidant in different solvents.



**Mehdi Masjedi, Tülin Demiralp, Saim Özkar***Journal of Molecular Catalysis A: Chemical* 310 (2009) 59

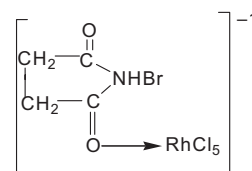
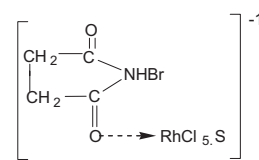
Testing catalytic activity of ruthenium(III) acetylacetonate in the presence of trialkylphosphite or trialkylphosphine in hydrogen generation from the hydrolysis of sodium borohydride

Catalytic activity of  $\text{Ru}(\text{acac})_3$  in the presence of different alkylphosphine ligands was investigated in the hydrolysis of sodium borohydride. Addition of phosphine leads to the formation of a species which has higher catalytic activity than  $\text{Ru}(\text{acac})_3$  alone. Varying the phosphine affects the catalytic activity and catalyst lifetime as well as the kinetics and activation parameters of the hydrolysis.

**Ashok Kumar Singh, Rashmi Srivastava, Shalini Srivastava, Jaya Srivastava, Shahla Rahmani, Bharat Singh***Journal of Molecular Catalysis A: Chemical* 310 (2009) 64

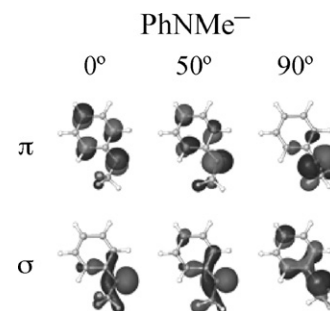
N-Bromosuccinimide oxidation of maltose and D-galactose using chloro-complex of Rh(III) in its nano-concentration range as homogeneous catalyst: A kinetic and mechanistic study

Kinetics of Rh(III)-catalysed oxidation of maltose and D-galactose by protonated NBS have been studied at 40 °C. A suitable reaction mechanism showing the formation of most reactive activated complex, by the interaction of a charged complex species and a neutral substrate molecule has been proposed.

**Hugo Vázquez-Lima, Patricia Guadarrama, Estrella Ramos, Serguei Fomine***Journal of Molecular Catalysis A: Chemical* 310 (2009) 75

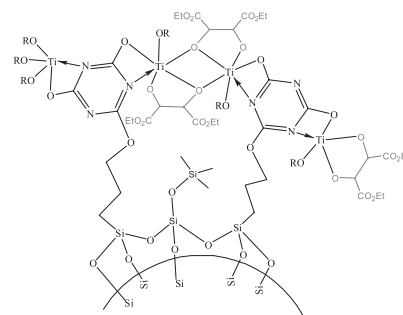
On the modulation of  $\text{N}_2$  activation from molecular orbitals viewpoint. Triamidoamine-Mo complexes as case of study

The understanding of what molecular orbitals are involved in the interaction Mo-catalyst- $\text{N}_2$  makes possible the modulation of such interaction by systematic rotations of the dihedral angles  $\text{Mo}-\text{N}_{\text{aryl}}-\text{C}_{\text{aryl}}$  to find an optimal geometry that weakens the N-N bond. The optimal geometry would be fixed by rigid dendritic scaffolds to construct a nitrogen-reducer macromolecular catalyst. DFT framework was used in the present study.

**Ruth Ballesteros, Mariano Fajardo, Isabel Sierra, Isabel del Hierro***Journal of Molecular Catalysis A: Chemical* 310 (2009) 83

Synthesis of titanium-triazine based MCM-41 hybrid materials as catalyst for the asymmetric epoxidation of cinnamyl alcohol

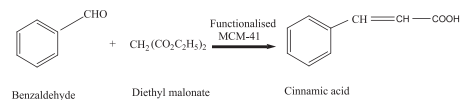
A molecular precursor approach involving tethering procedures was used to produce site isolated titanium-supported asymmetric epoxidation catalysts. This was done by first modifying the support in one step with a mixture of silanes: the synthesized triazine propyl triethoxysilane as functional linker and hexamethyldisilazane as capped agent, to increase the hydrophobicity of the support and mask the remaining silanol groups. In addition,  $[\text{Ti}(\text{OPr}^i)_4]$  and  $\{[\text{Ti}(\text{OPr}^i)_3(\text{OMent})]\}_2$  (MentO = 1R,2S,5R-(−)-mentho) complexes were heterogenized by reaction with the modified MCM-41. Finally, after  $[\text{Ti}(\text{OPr}^i)_4]$  immobilization on to the organomodified support the reaction with the chiral auxiliary (+)-diethyl-L-tartrate was accomplished. The different systems were tested in the asymmetric epoxidation of cinnamyl alcohol in order to evaluate their catalytic activity and enantioselectivity.



**K.M. Parida, Dharitri Rath***Journal of Molecular Catalysis A: Chemical* 310 (2009) 93

Amine functionalized MCM-41: An active and reusable catalyst for Knoevenagel condensation reaction

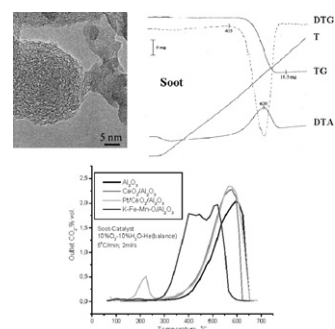
Amine modified MCM-41 can be used as reusable heterogeneous solid base catalyst for Knoevenagel condensation reaction at room temperature under solvent free condition. About 12.8 wt% amine modified MCM-41 prepared by co-condensation method showed highest malonic ester conversion (92%) and cinnamic acid selectivity (98%).



**Aleksandra S. Ivanova, Galina S. Litvak,  
Vladimir V. Mokrinskii, Lyudmila M. Plyasova,  
Vladimir I. Zaikovskii, Vasilii V. Kaichev,  
Aleksandr S. Noskov**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 101

The influence of the active component and support nature, gas mixture composition on physicochemical and catalytic properties of catalysts for soot oxidation

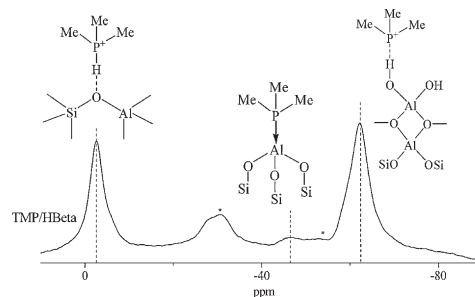


**Jing Guan, Xiujie Li, Gang Yang, Weiping Zhang,  
Xianchun Liu, Xiuwen Han, Xinhe Bao**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 113

Interactions of phosphorous molecules with the acid sites of H-Beta zeolite: Insights from solid-state NMR techniques and theoretical calculations

Acids play an important role in zeolite catalysis whereas their natures are currently under hot debates. With solid-state NMR techniques and theoretical calculations at various levels, two types of Brønsted acid sites and three types of Lewis acid sites in H-Beta zeolite were resolved. In addition, the interaction modes of TMP with all these acid sites were provided.

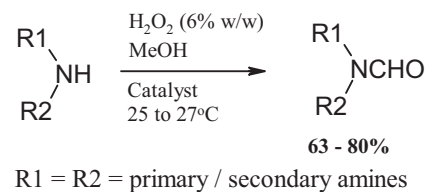


**Harikrishna Tumma, N. Nagaraju,  
K. Vijayakumar Reddy**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 121

A facile method for the N-formylation of primary and secondary amines by liquid phase oxidation of methanol in the presence of hydrogen peroxide over basic copper hydroxyl salts

Copper-based catalysts in the form of hydroxyl salts are effective in oxidation of methanol in the presence of dilute hydrogen peroxide to produce N-formylated amines from primary or secondary amines. Acid-sensitive functional groups can also be formylated in moderate to good yields.

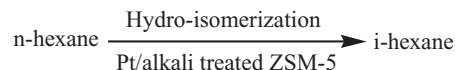


**Yue-Qin Song, Yan-Long Feng, Feng Liu,  
Cheng-Lin Kang, Xiao-Long Zhou, Long-Ya Xu,  
Guo-Xian Yu**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 130

Effect of variations in pore structure and acidity of alkali treated ZSM-5 on the isomerization performance

The alkali treatment to ZSM-5 had distinct effects on its acidity and pore structure and the n-hexane hydro-isomerization performance of Pt/ZSM-5. The mild alkali treatment led to a decrease in n-hexane conversion and selectivity for dimethylbutanes (DMB). However, the severe treatment enhanced n-hexane conversion and the selectivity for DMB.

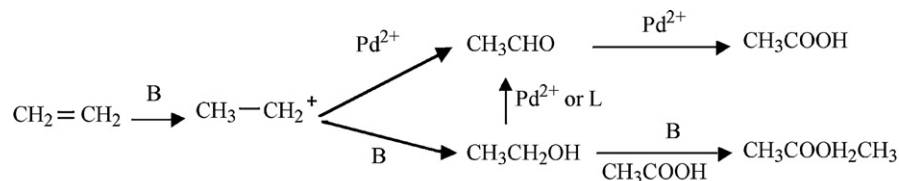


**Shuliang Xu, Lixia Wang, Wenling Chu,  
Weishen Yang**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 138

Influence of Pd precursors on the catalytic performance of Pd-H<sub>4</sub>SiW<sub>12</sub>O<sub>40</sub>/SiO<sub>2</sub> in the direct oxidation of ethylene to acetic acid

The effect of palladium precursors for Pd-H<sub>4</sub>SiW<sub>12</sub>O<sub>40</sub>/SiO<sub>2</sub> catalyst on the catalytic properties in the selective oxidation of ethylene to acetic acid has been investigated. The present study demonstrates that a well combination of Brönsted acid sites with dispersion of palladium is responsible for the catalytic activity.



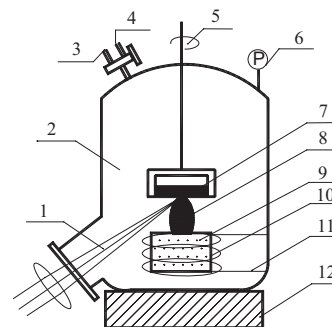
(B: Brönsted acid sites; L: Lewis acid sites; Pd<sup>2+</sup>: Pd<sup>2+</sup> species)

**Lingchao Jiang, Huizi Gu, Xingzhong Xu,  
Xinhuan Yan**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 144

Selective hydrogenation of o-chloronitrobenzene (o-CNB) over supported Pt and Pd catalysts obtained by laser vaporization deposition of bulk metals

The catalysts were prepared in the system of laser vaporization deposition. (1) Laser; (2) chamber; (3) N<sub>2</sub> cylinder; (4) vacuum pump; (5) stirrer; (6) vacuum meter; (7) metallic rod; (8) plasma; (9) support; (10) quartz dish; (11) strip heater; (12) magnetic stirrer.

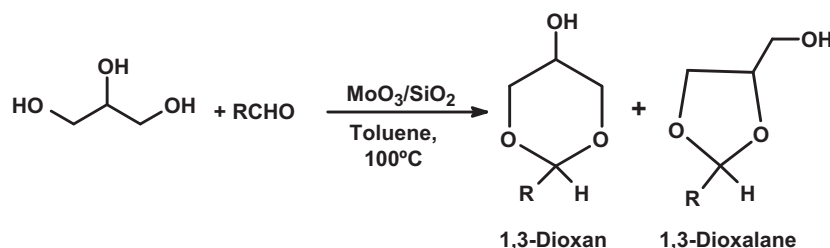


**Shubhangi B. Umbarkar, Trupti V. Kotbagi,  
Ankush V. Biradar, Renu Pasricha, Jyoti Chanale,  
Mohan K. Dongare, Anne-Sophie Mamede,  
Christine Lancelot, Edmond Payen**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 150

Acetalization of glycerol using mesoporous MoO<sub>3</sub>/SiO<sub>2</sub> solid acid catalyst

MoO<sub>3</sub>/SiO<sub>2</sub> catalysts prepared by sol-gel synthesis using ethyl silicate-40 was used for acetalization of glycerol with various aldehydes. Structural characterization showed the formation of molybdenum oxide nanoparticles of 1–2 nm on mesoporous silica support with very high acidity. Raman spectroscopy confirmed the presence of silicomolybdic acid, β-MoO<sub>3</sub>, polymolybdate and α-MoO<sub>3</sub> species with varying molybdenum content.

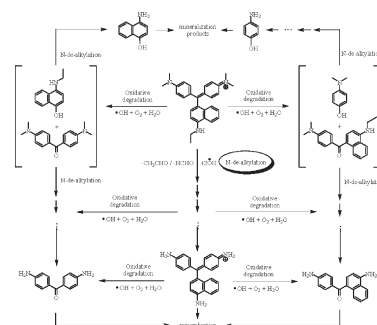


**Chungshin Lu, Yingtien Wu, Fuder Mai, Wenhsin Chung, Chiawei Wu, Wanyu Lin, Chiingchang Chen**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 159

Degradation efficiencies and mechanisms of the ZnO-mediated photocatalytic degradation of Basic Blue 11 under visible light irradiation

Because the same identified intermediates were obtained under UV or visible light irradiation, there is no doubt that the major oxidant under visible light irradiation is  $\cdot\text{OH}$  radical, not  $\text{O}_2^{\cdot-}$ . Both the *N*-de-ethylation and oxidative degradation of BB-11 take place in the presence of ZnO particles with visible light irradiation.

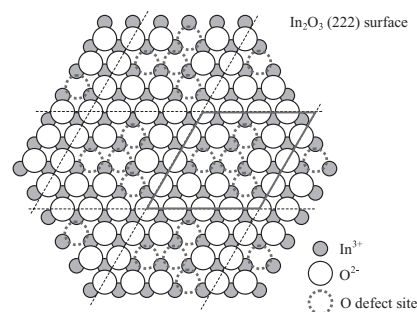


**Masaki Segawa, Satoshi Sato, Mika Kobune, Toshiaki Sodesawa, Takashi Kojima, Shin Nishiyama, Nobuo Ishizawa**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 166

Vapor-phase catalytic reactions of alcohols over bixbyite indium oxide

Vapor-phase catalytic reactions of several alcohols were investigated over  $\text{In}_2\text{O}_3$ .  $\text{In}_2\text{O}_3$  showed stable catalytic activity in the dehydration of terminal diols, such as 1,4-butanediol and 1,5-pentanediol, to produce selectively unsaturated alcohols, such as 3-buten-1-ol and 4-penten-1-ol, respectively. Redox sites around the oxygen defect sites of  $\text{In}_2\text{O}_3$  (2 2 2) plane are concluded to be active centers for the dehydration of diols to produce unsaturated alcohols.

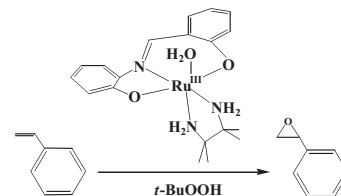


**Debabrata Chatterjee**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 174

Olefin epoxidation catalyzed by  $[\text{Ru}^{\text{III}}(\text{TDL})(\text{tmeda})\text{H}_2\text{O}]$  complexes (TDL = tridentate Schiff-base ligand; tmeda = tetramethylethylenediamine)

Mixed-chelate  $[\text{Ru}^{\text{III}}(\text{TDL})(\text{tmeda})(\text{H}_2\text{O})]$  (TDL = tridentate Schiff-base ligands and tmeda = tetramethylethylenediamine) complexes catalyze the epoxidation of alkenes effectively at ambient temperature using *t*-BuOOH as terminal oxidant. Based on Hammett correlation ( $\log k_{\text{rel}}$  vs.  $\Sigma^+$ ) and product analysis, intermediacy of a  $[\text{Ru}-\text{O}-\text{OBu}^t]$  radicaloid species is proposed for the catalytic epoxidation process.



**G.K. Surya Prakash, Juan C. Colmenares, Patrice T. Batamack, Thomas Mathew, George A. Olah**

*Journal of Molecular Catalysis A: Chemical* 310 (2009) 180

Poly(4-vinylpyridine) catalyzed hydrolysis of methyl bromide to methanol and dimethyl ether

The hydrolysis of methyl bromide with neutral water is performed in the presence and absence of various amines in a batch reactor at different temperatures (50–125 °C). Screening of poly(4-vinylpyridine) as a potential reusable solid amine catalyst showed maximum efficiency. This significant enhancement in efficiency is due to the capture of HBr by solid PVP and remains phase-separated driving the reaction forward. The major advantage of this process is that the polymer can be easily regenerated and reused without loss of activity making it a very effective catalyst for the conversion of methyl halides to methanol and dimethyl ether.

