



## Contents

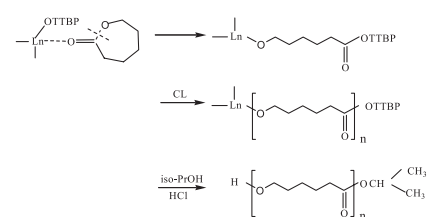
### Articles

**Lifang Zhang, Yanhui Niu, Yan Wang, Pei Wang, Lijuan Shen**

*Journal of Molecular Catalysis A: Chemical 287 (2008) 1*

Ring-opening polymerization of  $\epsilon$ -caprolactone by lanthanide tris(2,4,6-tri-*tert*-butylphenolate)s: Characteristics, kinetics and mechanism

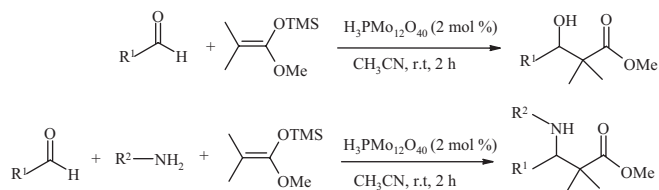
The end group analyses on prepared polymer demonstrate that the ring-opening polymerization of  $\epsilon$ -caprolactone with lanthanum tris(2,4,6-tri-*tert*-butylphenolate)s in toluene proceeds via a coordination–insertion mechanism. The monomer coordinated to rare earth metal, and opened its ring via acyl-oxygen bond cleavage forming a growing chain. The following monomer repeated these steps to insert into the Ln–O bond in the propagation process.



**Akbar Heydari, Samad Khaksar, Mehdi Sheykhani, Mahmoud Tajbaksh**

*Journal of Molecular Catalysis A: Chemical 287 (2008) 5*

$H_3PMo_{12}O_{40}$  as a new and reusable catalyst for Mukaiyama and Mannich reactions in heterogeneous media

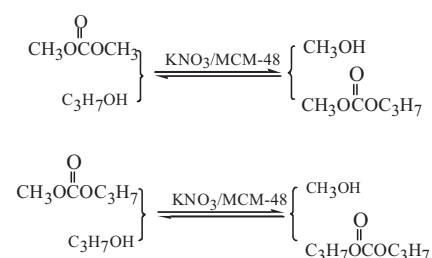


**Yongxin Li, Yanhua Zhang, Bing Xue, Yuhua Guo**

*Journal of Molecular Catalysis A: Chemical 287 (2008) 9*

Synthesis of dipropyl carbonate by transesterification over  $KNO_3$ /MCM-48

$KNO_3$ /MCM-48 exhibited very high catalytic activity under the optimized reaction conditions. Its characterization revealed that the highest catalytic activity of  $KNO_3$ /MCM-48 was probably due to the completely decomposition of  $KNO_3$  and the formation of active sites at high calcination temperature. The effects of reaction conditions on the performance of the catalyst and the mechanism of transesterification were discussed.

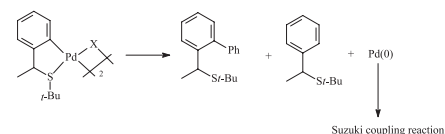


**Danilo Zim, Sabrina M. Nobre, Adriano L. Monteiro**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 16

Suzuki cross-coupling reaction catalyzed by sulfur-containing palladacycles: Formation of palladium active species

Sulfur-containing palladacycles were studied mechanistically in the Suzuki reaction. The catalytic reaction was monitored by  $^{19}\text{F}$  NMR and GC-MS and the decomposition of the S-palladacycle was studied under stoichiometric conditions, showing that these palladacycles served as a reservoir of zerovalent palladium species. Poisoning studies and transmission electron microscopy analysis results indicated the presence of small palladium nanoparticles ( $3.3 \pm 0.8$  nm). Competitive experiments provide evidence that sulfur-containing palladacycle and  $\text{PdCl}_2(\text{SEt}_2)_2$  form the same active species in the oxidative addition step in Suzuki reactions and that these species are equivalent to those for the Heck reaction using the same palladacycle.

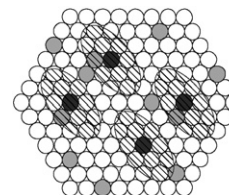


**María I. Cabrera, Ricardo J. Grau**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 24

Methyl oleate isomerization and hydrogenation over  $\text{Ni}/\alpha\text{-Al}_2\text{O}_3$ : A kinetic study recognizing differences in the molecular size of hydrogen and organic species

The kinetics of the *cis-trans* isomerization and hydrogenation of methyl oleate on a  $\text{Ni}/\alpha\text{-Al}_2\text{O}_3$  catalyst was studied in the absence of mass-transport limitation, at  $398\text{K} \leq T \leq 443\text{K}$  and  $370\text{kPa} \leq P_{\text{H}_2} \leq 650\text{kPa}$ . Results and distinctive features characterizing the kinetic modeling based on the advanced concept of semi-competitive adsorption model are highlighted. Adsorbed molecule of methyl oleate could cover up to seven surface sites.

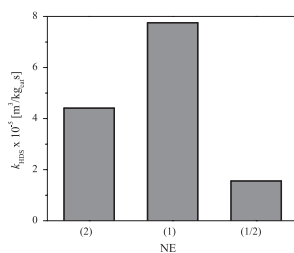


**J. Escobar, M.C. Barrera, J.A. de los Reyes, J.A. Toledo, V. Santes, J.A. Colín**

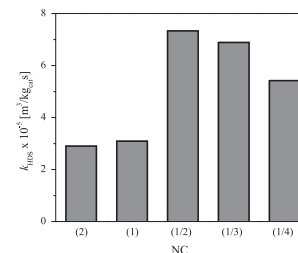
*Journal of Molecular Catalysis A: Chemical* 287 (2008) 33

Effect of chelating ligands on Ni-Mo impregnation over wide-pore  $\text{ZrO}_2\text{-TiO}_2$

Dibenzothiophene hydrodesulfurization activity of sulfided  $\text{NiMo}/\text{ZrO}_2\text{-TiO}_2$  catalysts impregnated at various Ni/EDTA (NE) ratios. Operating conditions: batch reactor,  $T = 320^\circ\text{C}$ ,  $P = 5.72$  MPa, *n*-hexadecane as solvent, 1000 rpm, mixing speed.



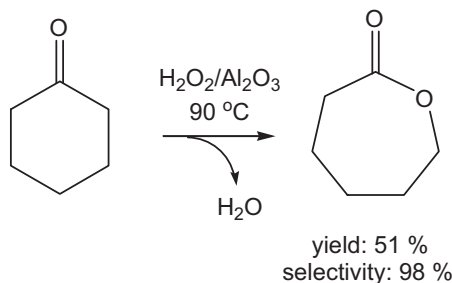
Dibenzothiophene hydrodesulfurization activity of sulfided  $\text{NiMo}/\text{ZrO}_2\text{-TiO}_2$  catalysts impregnated at various Ni/citric acid (NC) ratios. Operating conditions: batch reactor,  $T = 320^\circ\text{C}$ ,  $P = 5.72$  MPa, *n*-hexadecane as solvent, 1000 rpm, mixing speed.



**Rafael Augusto Steffen, Sergio Teixeira, Jorge Sepulveda, Roberto Rinaldi, Ulf Schuchardt**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 41

Alumina-catalyzed Baeyer-Villiger oxidation of cyclohexanone with hydrogen peroxide

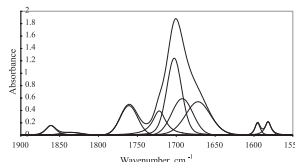


**Yury V. Kissin, Xinsheng Liu, David J. Pollick,  
Nancy L. Brungard, Main Chang**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 45

Ziegler-Natta catalysts for propylene polymerization: Chemistry of reactions leading to the formation of active centers

The article describes chemical reactions between a fourth-generation solid Ziegler-Natta catalyst for propylene polymerization,  $\text{TiCl}_4/\text{MgCl}_2/\text{diisobutyl phthalate (DIBP)}$ , and cocatalyst mixtures containing  $\text{AlEt}_3$  and  $(\text{Cy})(\text{Me})\text{Si}(\text{OMe})_2$ . The reactions result in a significant reduction of the amounts of all carbonyl species present in the original solid catalyst (complexes of DIBP with  $\text{MgCl}_2$  and  $\text{TiCl}_4$  and complexes of  $\text{MgCl}_2$  with phthaloyl chloride formed in the process of catalyst synthesis), and in the reduction of surface  $\text{Ti}^{\text{IV}}$  species to  $\text{Ti}^{\text{III}}$ . Components of the cocatalyst mixture, including complexes of  $(\text{Cy})(\text{Me})\text{Si}(\text{OMe})_2$  with  $\text{AlEt}_3$ , are strongly adsorbed on the surface of the solid catalyst and on the surface of the products of its reactions with excess  $\text{AlEt}_3$ . The most probable coordination site for  $(\text{Cy})(\text{Me})\text{Si}(\text{OMe})_2$  is the surface Ti species, including active centers in olefin polymerization reactions. Carbonyl species in solid catalyst prior to its interaction with cocatalyst mixture.

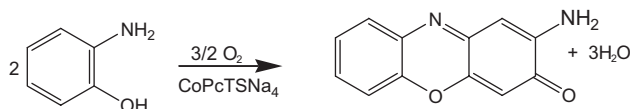


**M. Hassanein, M. Abdo, S. Gerges, S. El-Khalafy**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 53

Study of the oxidation of 2-aminophenol by molecular oxygen catalyzed by cobalt(II) phthalocyaninetetrasodiumsulfonate in water

Cobalt(II) phthalocyaninetetrasodiumsulfonate has been found to enhance the rate of oxidation of 2-aminophenol with dioxygen in water to 2-amino-phenoxazin-3-one. The oxidation reaction was followed by measuring dioxygen uptake. The rate constants of oxidation reaction showed linear dependence on catalyst concentration and saturation kinetics in both 2-aminophenol concentration and dioxygen pressure.

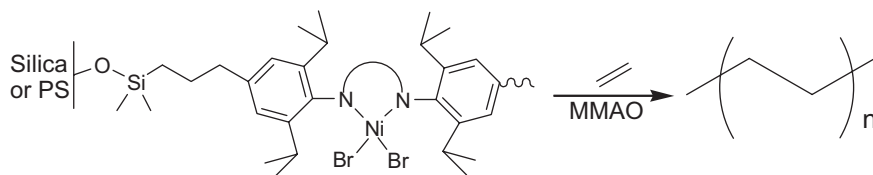


**Yan-Guo Li, Li Pan, Zhan-jiang Zheng, Yue-Sheng Li**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 57

Polymerization of ethylene to branched polyethylene with silica and Merrifield resin supported nickel(II) catalysts with  $\alpha$ -diimine ligands

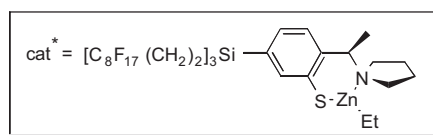
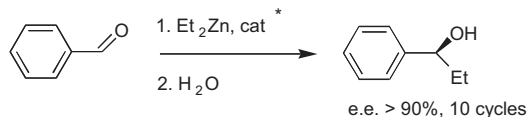
$\alpha$ -Diimine nickel(II) complexes have been immobilized on silica and Merrifield resin. The supported catalysts were used for ethylene polymerization in the presence of MMAO, yielding branched polyethylenes with high molecular weight.



**Henk Kleijn, Johann T.B.H. Jastrzebski,  
Berth-Jan Deelman, Gerard van Koten**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 65

Efficient recycling of fluororous versions of highly enantioselective *S,N*-chelated zinc aminoarene thiolate catalysts for the 1,2-addition of diethylzinc to benzaldehydes

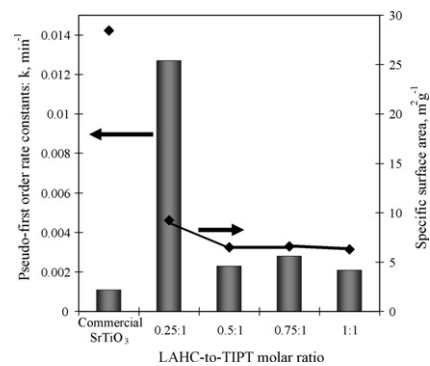


**Tarawipa Puangpetch, Thammanoon Sreethawong, Susumu Yoshikawa, Sumaeth Chavadej**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 70

Synthesis and photocatalytic activity in methyl orange degradation of mesoporous-assembled SrTiO<sub>3</sub> nanocrystals prepared by sol-gel method with the aid of structure-directing surfactant

The main objective of this work is to reveal a newly developed synthesis procedure for mesoporous-assembled SrTiO<sub>3</sub> nanocrystal photocatalyst using a sol-gel process combined with structure-directing surfactant. The obtained photocatalyst exhibited much higher photocatalytic activity for degradation of methyl orange, used as a model azo dye pollutant in wastewater, than commercially available SrTiO<sub>3</sub> nanopowder.

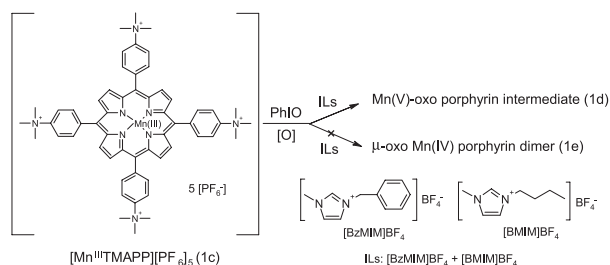


**Hong-Jiao Zhang, Ye Liu, Yong Lu, Xiao-Shuang He, Xia Wang, Xia Ding**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 80

Epoxidations catalyzed by an ionic manganese(III) porphyrin and characterization of manganese(V, IV)-oxo porphyrin complexes by UV-vis spectrophotometer in ionic liquid solution

The compositions of an ionic manganese porphyrin (1c) resided in the ionic liquids were applied triply as the catalyst, the axial ligand, and the solvent for epoxidations of styrene (derivatives) with advantages of high efficiency, suppressed oxidation destruction of the porphyrin itself, and dramatically improved stability of the active Mn(V)-oxo porphyrin intermediate.

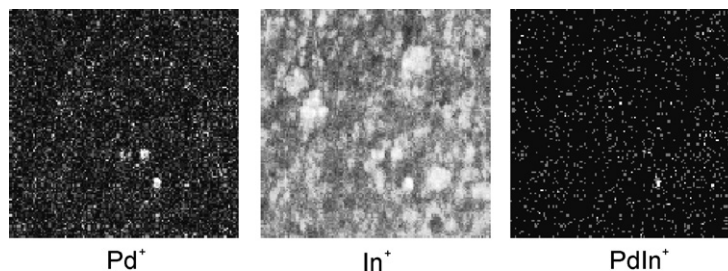


**I. Witońska, S. Karski, J. Rogowski, N. Krawczyk**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 87

The influence of interaction between palladium and indium on the activity of Pd-In/Al<sub>2</sub>O<sub>3</sub> catalysts in reduction of nitrates and nitrites

Bimetallic Pd-In/Al<sub>2</sub>O<sub>3</sub> catalysts are characterized by high activity in the reduction of nitrates and nitrites. However, systems containing the largest amount of indium (5%Pd-5%In/Al<sub>2</sub>O<sub>3</sub>) show poorer activity in the studied reactions. On the basis of our investigations, we can say that there are two effects which can influence activity of Pd-In/Al<sub>2</sub>O<sub>3</sub> catalysts in the reduction of nitrates and nitrites: the formation of intermetallic phase and/or the increase in indium surface concentrations in those bimetallic systems.



**Arno Behr, Guido Henze, Leif Johnen, Sebastian Reyer**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 95

Selective catalytic formation of unsaturated amino acids from petrochemicals and carbon dioxide—Application of high-throughput catalyst screening

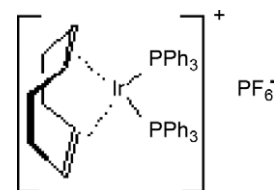
The homogeneous catalytic 1,4-hydroamination of the 2-ethylidene-6-heptene-5-olide ( $\delta$ -lactone), obtained by the telomerisation of easily accessible 1,3-butadiene and the green house gas carbon dioxide, is described, yielding an amino acid in a single step. A new reactor concept is introduced which allows practical high-throughput catalyst screening with low costs.



**Silke Taubmann, Helmut G. Alt***Journal of Molecular Catalysis A: Chemical* 287 (2008) 102

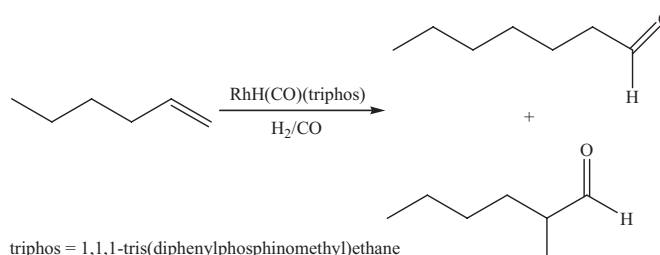
Heterogeneous catalysts for the dehydrogenation of saturated hydrocarbons

A series of new heterogeneous iridium containing catalysts was synthesized by the incipient wetness method. The used support materials were  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{TiO}_2$ ,  $\text{ZrO}_2$ , and MCM-41.

**Merlín Rosales, Gustavo Chacón, Angel González, Inés Pacheco, Pablo J. Baricelli, Luis G. Melean***Journal of Molecular Catalysis A: Chemical* 287 (2008) 110

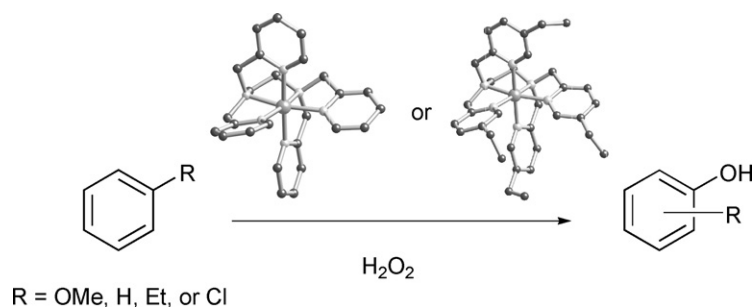
Kinetics and mechanisms of homogeneous catalytic reactions. Part 9. Hydroformylation of 1-hexene catalyzed by a rhodium system containing a tridentated phosphine

The system  $\text{Rh}(\text{acac})(\text{CO})_2/\text{triphos}$  is an efficient precatalyst for the homogeneous hydroformylation of 1-hexene under mild reaction conditions; the linear to branched ratio ( $l/b$ ) of aldehydes formed varied between 1.3 and 5.8 and it is dependent on the reaction conditions. Kinetic and mechanistic studies allowed us to propose a catalytic cycle, in which  $\text{RhH}(\text{CO})(\kappa^3\text{-triphos})$  is the resting state of the catalyst and the insertion of the alkene into the metal-hydride bond is the rate-determining step.

**Aurore Thibon, Jean-François Bartoli, Régis Guillot, Joëlle Sainton, Marlène Martinho, Daniel Mansuy, Frédéric Banse***Journal of Molecular Catalysis A: Chemical* 287 (2008) 115

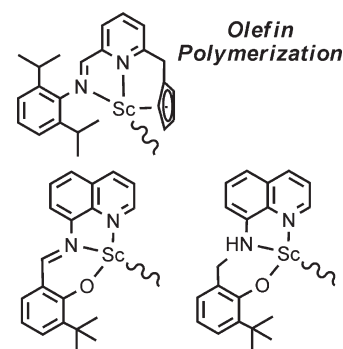
Non-heme iron polyazadentate complexes as catalysts for aromatic hydroxylation by  $\text{H}_2\text{O}_2$ : Particular efficiency of tetrakis(2-pyridylmethyl) ethylenediamine-iron(II) complexes

Two Fe(II) complexes with hexaazadentate ligands were prepared, characterized and compared as catalysts for the hydroxylation of aromatic substrates. One of these complexes gave the best yields ever reported for such coordination complexes.

**Gino Paolucci, Marco Bortoluzzi, Mariagrazia Napoli, Pasquale Longo***Journal of Molecular Catalysis A: Chemical* 287 (2008) 121

Scandium complexes with [N,N,Cp] and [N,N,O] donor set ancillary ligands as catalysts in olefin polymerization

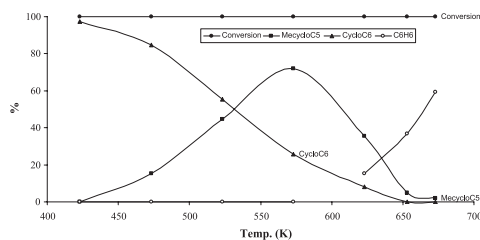
New Sc(III) chloro-complexes with anionic polydentate [N,N,Cp] and [N,N,O] donor sets ligands  $[\text{ScCl}_2(\text{NNCp})(\text{THF})]$ ,  $[\text{ScCl}_2(\text{NNO})(\text{THF})]$  and  $[\text{ScCl}_2(\text{NNHO})(\text{THF})]$  have been synthesized and characterized by NMR and mass spectrometry. The comparative results of their behavior as catalytic precursors in ethylene and butadiene polymerization are reported and explained on the basis of the electronic and steric properties of the ancillary ligands.



**H. Al-Kandari, F. Al-Kharafi, A. Katrib***Journal of Molecular Catalysis A: Chemical* 287 (2008) 128

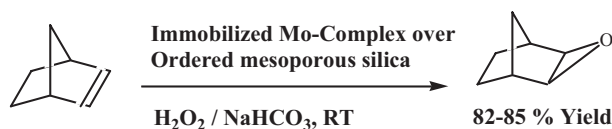
Catalytic activity-surface structure correlation of molybdenum-based catalysts

Controlled reduction at 673 and 873 K of the equivalent 5 monolayer of molybdenum trioxide deposited on  $\text{TiO}_2$  enabled us to obtain two distinct, well-defined bifunctional  $\text{MoO}_2(\text{H}_x)_{\text{ac}}$  and  $\text{Mo}(0)$  states of molybdenum surfaces as characterized by XPS-UPS and HRTEM techniques. Catalytic reactions of *n*-hexane, 1-hexene, cyclohexene and cyclohexane were studied using both catalytic systems. Different catalytic reactions on both surfaces were found to be reaction temperature, electronic and surface structure dependent.

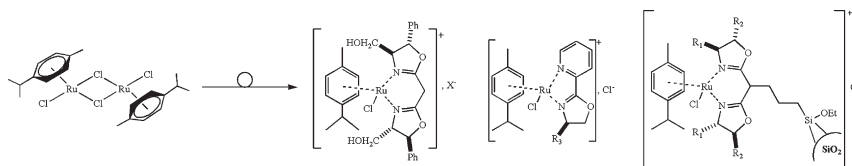
**Swarup K. Maiti, Subhajit Dinda, Mahasweta Nandi, Asim Bhaumik, Ramgopal Bhattacharyya***Journal of Molecular Catalysis A: Chemical* 287 (2008) 135

Selective epoxidation of olefins catalyzed by oxodiperoxomolybdenum(VI) complexes immobilized over highly ordered 2D-hexagonal mesoporous silica

Neutral and anionic oxodiperoxo-8-quinolinolato Mo(VI) complexes have been immobilized over highly ordered 2D-hexagonal mesoporous silica. These immobilized catalysts showed excellent activity and recycling efficiency in one pot liquid phase selective oxidation of bulky olefins by using dilute aqueous  $\text{H}_2\text{O}_2$  as oxidant.

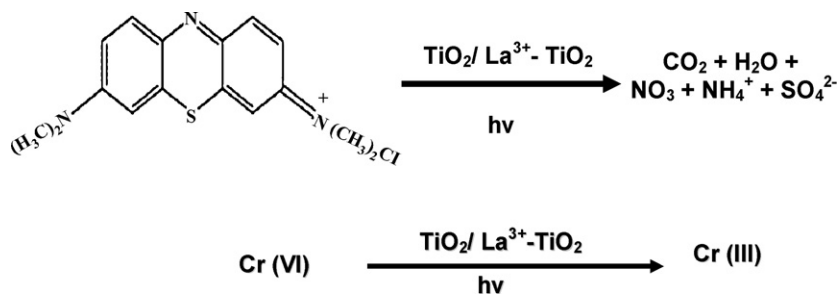
**Nathalie Debono, Catherine Pinel, Rabih Jahjah, Ali Alaaeddine, Pierre Delichère, Frédéric Lefebvre, Laurent Djakovitch***Journal of Molecular Catalysis A: Chemical* 287 (2008) 142

Asymmetric reduction of ketones with ruthenium-oxazoline based catalysts

**K.M. Parida, Nruparaj Sahu***Journal of Molecular Catalysis A: Chemical* 287 (2008) 151

Visible light induced photocatalytic activity of rare earth titania nanocomposites

Doping of  $\text{Ln}^{3+}$  on  $\text{TiO}_2$  increases the photocatalytic reaction; 80% of methylene blue (MB) degradation and 86.5% of Cr (VI) reduction were found in case of 0.4 mol%  $\text{La}^{3+}$  doped  $\text{TiO}_2$  against 30% of MB degradation and 45% of Cr (VI) reduction incase of neat  $\text{TiO}_2$ .

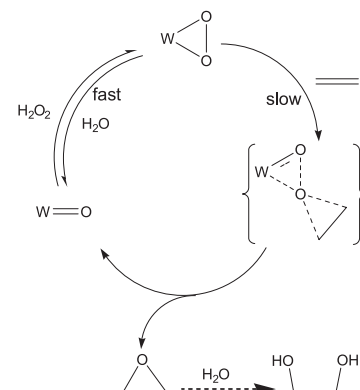


**Ahmad M. Al-Ajlouni, Özgül Sağlam, Tariq Diafla, Fritz E. Kühn**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 159

Kinetic studies on phenylphosphopolyperoxotungstates catalyzed epoxidation of olefins with hydrogen peroxide

The catalytic activities of phenylphosphopolyperoxotungstates for the epoxidation of alkenes and styrenes by  $H_2O_2$  have been investigated under homogeneous and biphasic conditions. The presence of an electron-withdrawing group, such as nitro, increases the epoxidation rate as well as the epoxide ring-opening.

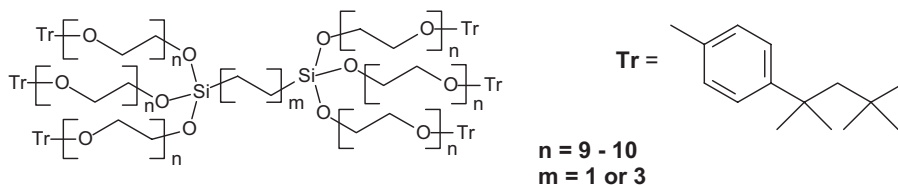


**Bogusława Łęska, Radosław Pankiewicz, Błażej Gierczyk, Grzegorz Schroeder**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 165

Synthesis, structure and application of a new class of Tr-podands derived in phase-transfer catalysis

In this paper we reported the first synthesis of the group of Triton polypodands, characterized by different central atoms, such as Si, B or P. Results of this study demonstrate the potential of these compounds in some organic reactions in phase-transfer catalysis (PTC) conditions. The catalytic activity of Triton X (**1**) and Tr-podands (**2–8**) has been evaluated in an ion promoted reaction under solid-liquid phase-transfer catalysis conditions and compared with that of the earlier studied Si-podands (**9–11**).

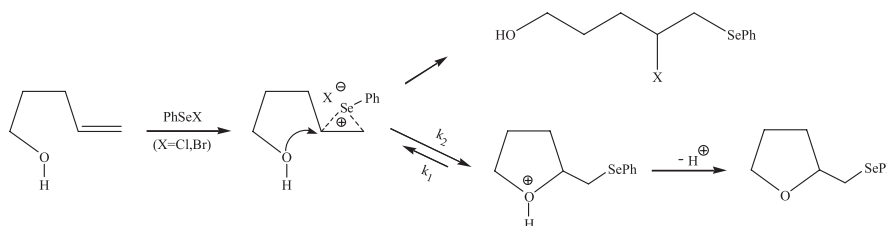


**Zorica M. Bugarčić, Biljana V. Petrović, Marina D. Rvović**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 171

Kinetics and mechanism of the pyridine-catalyzed reaction of phenylselenenyl halides and some unsaturated alcohols

The kinetics and mechanism of the reaction of phenylselenenyl halides ( $PhSeX$ ,  $X = Cl, Br$ ) and some primary unsaturated alcohols (pent-4-en-1-ol and hex-5-en-1-ol) in tetrachloromethane media have been studied, as the *pseudo*-first order, in the presence and absence of pyridine as catalyst by variable temperature UV-vis spectrophotometry. The negative values for entropy of activation for all studied reactions confirm the  $S_N2$  mechanism of substitution.



**Haiqiang Wang, Zhongbiao Wu, Yue Liu, Zhongyi Sheng**

*Journal of Molecular Catalysis A: Chemical* 287 (2008) 176

The characterization of ZnO-anatase-rutile three-component semiconductor and enhanced photocatalytic activity of nitrogen oxides

Three-component semiconductors just like ZnO-anatase-rutile with different zinc ion content (between 0.1 and 10.0 at%) were prepared by a wet impregnation method and investigated with respect to their behavior in UV photocatalytic oxidation of nitric oxide. Firstly, it was found that the  $OH^-$  species were improved on the surface of ZnO-anatase-rutile three-component system, which was favorable for the oxidation of NO by interrupting the formation of adsorbed nitrolysis. Secondly, the lifetime of electrons and holes was prolonged and the enhancement of the photocatalytic activity was observed for the  $Zn^{2+}$  doping concentration ranged from 0.1 to 2.0 at%.

