



## Contents

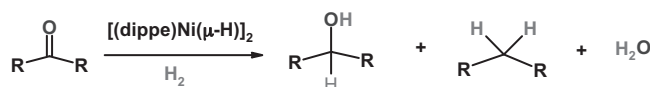
### Articles

**Areli Flores-Gaspar, Paulina Pinedo-González, Marco G. Crestani, Miguel Muñoz-Hernández, David Morales-Morales, Brian A. Warsop, William D. Jones, Juventino J. García**

*Journal of Molecular Catalysis A: Chemical 309 (2009) 1*

Selective hydrogenation of the C=O bond of ketones using Ni(0) complexes with a chelating bisphosphine

The reduction of ketones and diketones to yield an alcohol or alkane can be selectively achieved with nickel complexes and properly selecting the reaction conditions.

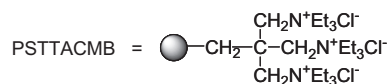
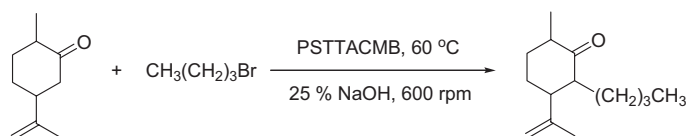


**Eagambaram Murugan, Prakash Gopinath**

*Journal of Molecular Catalysis A: Chemical 309 (2009) 12*

Triphase catalytic activity of a new insoluble multi-site phase transfer catalyst in C-alkylation of dihydrocarvone—A kinetic study

New insoluble multi-site phase transfer catalyst containing three active sites was synthesized, characterized and catalytic activity was determined through C-alkylation of dihydrocarvone using NaOH (25%, w/w) at 60 °C.

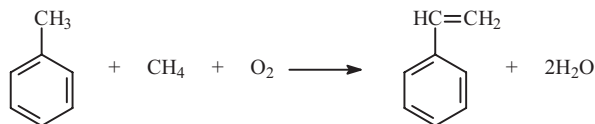


**Juan Carlos Colmenares, Jacek Kijenski, Enzo B. Arévalo-García**

*Journal of Molecular Catalysis A: Chemical 309 (2009) 21*

Chemical trapping studies to the determination of surface species under reaction conditions for the catalytic side-chain oxidative alkylation of toluene by methane

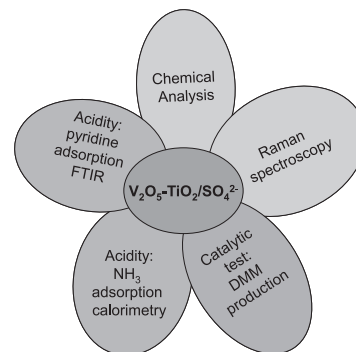
MgO-modified with Na and Cs ions have been studied for the side-chain oxidative methylation of toluene to ethylbenzene and styrene at 750 °C and atmospheric pressure. Chemical trapping has been a very useful technique to identify the adsorbed species on the catalyst surface under the reaction conditions. Chemical trapping and catalysts strong mono-electron-donor studies are very good experimental evidence of the radical mechanism in this reaction.



**H. Zhao, S. Bennici, J. Shen, A. Auroux***Journal of Molecular Catalysis A: Chemical* 309 (2009) 28

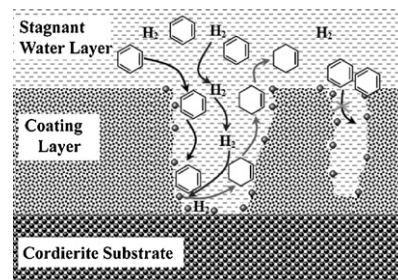
Surface and catalytic properties of  $V_2O_5$ - $TiO_2/SO_4^{2-}$  catalysts for the oxidation of methanol prepared by various methods

The influence of the preparation method on the surface and catalytic properties of sulfated vanadia-titania catalysts prepared by co-precipitation, sol-gel and mechanical grinding methods have been studied. After characterization by complementary techniques the catalysts were tested in the production of dimethoxymethane (DMM) by selective oxidation of methanol.

**Yujun Zhao, Jin Zhou, Jianguo Zhang, Shudong Wang***Journal of Molecular Catalysis A: Chemical* 309 (2009) 35

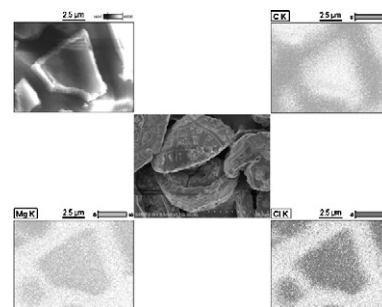
Liquid-phase selective hydrogenation of benzene to cyclohexene on  $Ru/Al_2O_3-ZrO_2/cordierite$  monolithic catalysts

$Ru/Al_2O_3-ZrO_2/cordierite$  monolithic catalysts were found to be an efficient catalyst for liquid-phase selective hydrogenation of benzene to cyclohexene in a fix-bed reactor. High cyclohexene yield was achieved on the coating layer, where the consecutive hydrogenation of cyclohexene to cyclohexane was readily prohibited.

**Hanna-Leena Rönkkö, Tarmo Korpela, Hilkka Knuuttila, Tuula T. Pakkanen, Peter Denifl, Timo Leinonen, Marianna Kemell, Markku Leskelä***Journal of Molecular Catalysis A: Chemical* 309 (2009) 40

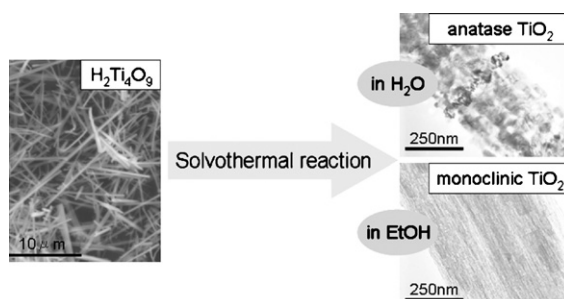
Particle growth and fragmentation of solid self-supported Ziegler-Natta-type catalysts in propylene polymerization

The article describes fragmentation studies on solid Ziegler-Natta-type catalysts prepared via emulsion technique. Propylene gas-phase polymerizations in a micro-reactor were carried out with different polymerization times and compared with corresponding polymerizations carried out with the conventional  $MgCl_2$ -supported Ziegler-Natta catalyst. Fragmentation morphology of the catalyst particles was studied by SEM/EDS. Fragmentation of the catalyst starts at the very beginning of the polymerization and proceeds with increasing polymerization time. Fragments of the emulsion-based catalyst are detected as plates (figure) on the surface of the polymer particles.

**Peilin Zhang, Shu Yin, Valery Petrykin, Masato Kakihana, Tsugio Sato***Journal of Molecular Catalysis A: Chemical* 309 (2009) 50

Preparation of high performance fibrous titania photocatalysts by the solvothermal reaction of protonated form of tetratitanate

By the solvothermal reaction of  $H_2Ti_4O_9$ , fibrous  $TiO_2$  with different crystalline phases, and fibrous structures were obtained, which showed high photocatalytic activity for the oxidative photodestruction of NO gas.

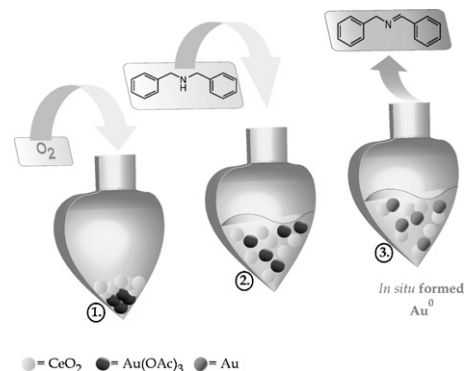


**Linda Aschwanden, Tamas Mallat,  
Frank Krumeich, Alfons Baiker**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 57

A simple preparation of an efficient heterogeneous gold catalyst for aerobic amine oxidation

For the oxidation of amines a very simple preparation of a heterogeneous gold catalyst has been developed. The catalyst has a comparable or even superior activity compared to other formerly published or commercially available catalysts.

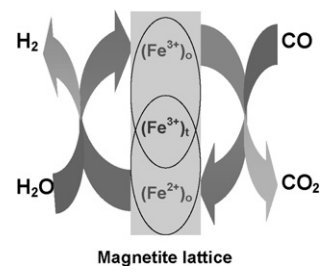


**Lingzhi Zhang, Jean-Marc M. Millet,  
Umit S. Ozkan**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 63

Deactivation characteristics of Fe–Al–Cu water-gas shift catalysts in the presence of H<sub>2</sub>S

This article reports the effect of H<sub>2</sub>S exposure on the Fe-based water-gas shift catalysts and the surface and structural changes upon deactivation. A mechanism for catalyst deactivation with H<sub>2</sub>S was proposed by combining the reaction testing and characterization results.

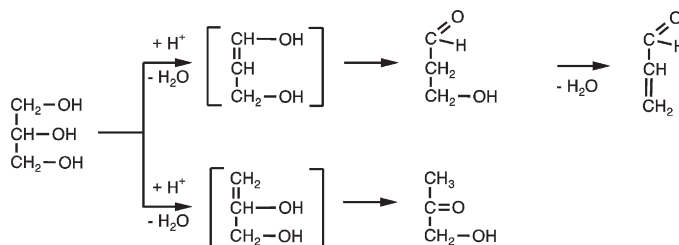


**Wladimir Suprun, Michal Lutecki, Thomas Haber,  
Helmut Papp**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 71

Acidic catalysts for the dehydration of glycerol: Activity and deactivation

The gas-phase dehydration of glycerol in presence of water was investigated at 280 °C. Glycerol conversion and acrolein selectivity depended on the total acidity and on the textural properties. Additionally, the formation of by-products during the dehydration of glycerol and the conversion of 1-hydroxyacetone and 3-hydroxypropionaldehyde catalysts was studied.

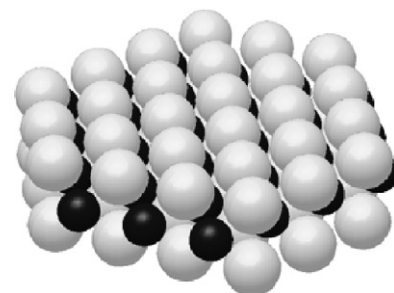


**Bas M. Vogelaar, Narinobu Kagami,  
Thomas F. van der Zijden, A. Dick van Langeveld,  
Sonja Eijsbouts, Jacob A. Moulijn**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 79

Relation between sulfur coordination of active sites and HDS activity for Mo and NiMo catalysts

The structure of Mo and NiMo HDS catalysts was studied using IR analysis of adsorbed CO. The Type II NiMo catalyst had a fully promoted structure, whereas the Type I NiMo catalyst exhibited both promoted and unpromoted sites. An inverse correlation was found between thiophene conversion and the number of vacant sites present on the catalyst surface. A similar trend was observed for the ratio between hydrogenation and direct desulfurization of dibenzothiophene, showing that the hydrogenation pathway is catalyzed by sulfided species on the active phase, while the direct desulfurization pathway is catalyzed by vacant sites.

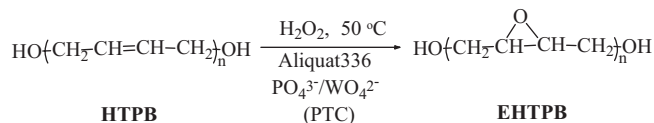


**Qingfa Wang, Xiangwen Zhang, Li Wang, Zhentao Mi**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 89

Epoxidation of hydroxyl-terminated polybutadiene with hydrogen peroxide under phase-transfer catalysis

The epoxidized HTPB was successfully and efficiently synthesized by epoxidation of HTPB with 34 wt% H<sub>2</sub>O<sub>2</sub> in presence of quaternary ammonium salts as the phase-transfer catalyst, ammonium tungstate hydrate and 85 wt% phosphoric acid as the epoxidation cocatalyst, and an auxiliary organic solvent.

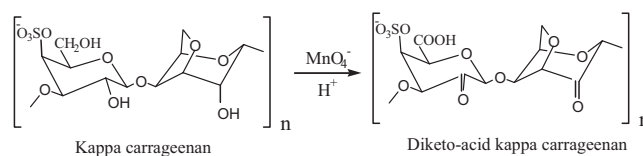


**R.M. Hassan, A. Fawzy, G.A. Ahmed, I.A. Zaafarany, B.S. Asghar, K.S. Khairou**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 95

Acid-catalyzed oxidation of some sulfated macromolecules. Kinetics and mechanism of oxidation of kappa-carrageenan polysaccharide by permanganate ion in acid perchlorate solutions

The product of oxidation of kappa-carrageenan by acidic permanganate (DKA-KCAR) has been elucidated by microanalysis and IR spectroscopy.

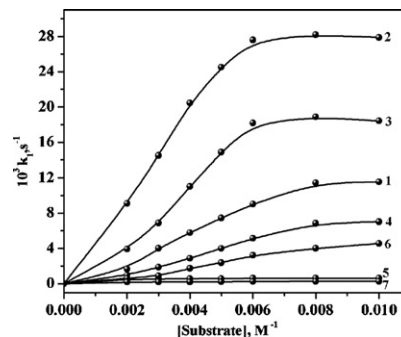


**A. Mary Imelda Jayaseeli, S. Rajagopal**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 103

[Iron(III)-salen] ion catalyzed H<sub>2</sub>O<sub>2</sub> oxidation of organic sulfides and sulfoxides

Iron(III)-salen complexes catalyze the H<sub>2</sub>O<sub>2</sub> oxidation of aryl methyl sulfides and sulfoxides. The reaction follows Michaelis-Menten kinetics and the rate of the reaction is influenced by the change of substituents in the aryl moiety of ArSMe or ArS(O)Me and phenolic moiety of the salen ligand. The product analyses show selective oxidation of sulfides to sulfoxides and sulfoxides to sulfones. Based on the kinetic and spectral studies the possible mechanisms are proposed.

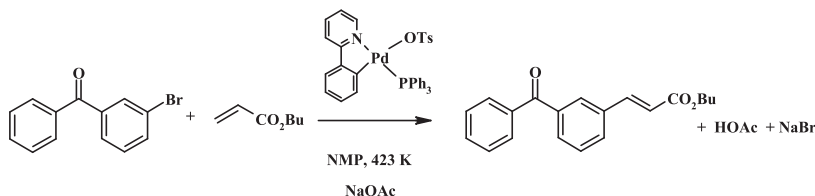


**Shashi B. Atla, Kalpendra B. Rajurkar, Ashutosh A. Kelkar, Raghunath V. Chaudhari**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 111

Kinetics of arylation of 3-bromo-benzophenone with *n*-butylacrylate using NC palladacycle catalyst

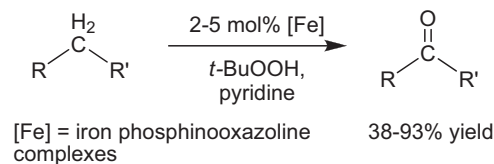
The kinetics of arylation of *n*-butylacrylate with 3-bromo-benzophenone (BBP) using a monomeric palladacycle complex catalyst has been studied. Effect of reaction conditions on initial rate of the reaction was investigated. Various empirical rate equations were considered to fit the rate data and the best fitting model has been selected.



**Matthew Lenze, Eike B. Bauer***Journal of Molecular Catalysis A: Chemical* 309 (2009) 117

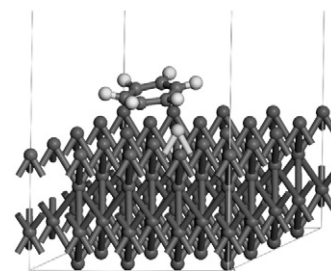
Oxidation of activated methylene groups to ketones catalyzed by new iron phosphinoxazoline complexes and by iron(II) triflate

Novel iron phosphinoxazoline complexes were synthesized and their catalytic activity in the oxidation of benzylic methylene groups was investigated. At a catalyst load from 2 to 5%, isolated yields ranged from 38 to 93%. The reaction presumably proceeds through a Fenton type mechanism and is pseudo zero order in substrate.

**Pei-Qing Yuan, Bing-Qiang Wang, Yue-Ming Ma, Hui-Min He, Zhen-Min Cheng, Wei-Kang Yuan***Journal of Molecular Catalysis A: Chemical* 309 (2009) 124

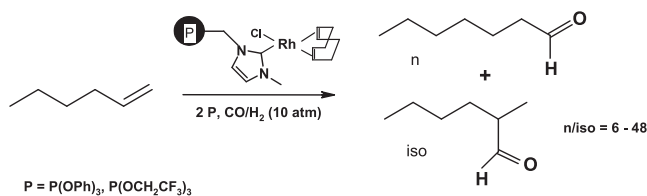
Partial hydrogenation of benzene over the metallic Zn modified Ru-based catalyst

From the adsorption point of view, partial hydrogenation of benzene over metallic Zn modified Ru-based catalyst was investigated. Theoretical calculation suggests that chemisorption of benzene and cyclohexene on the modified catalyst is both restrained, and the latter is much more serious than the former. A reduced catalytic activity but improved selectivity to cyclohexene therefore is experimentally observed.

**Wojciech Gil, Katarzyna Boczoń, Anna M. Trzeciak, Józef J. Ziółkowski, Eduardo Garcia-Verdugo, Santiago V. Luis, Victor Sans***Journal of Molecular Catalysis A: Chemical* 309 (2009) 131

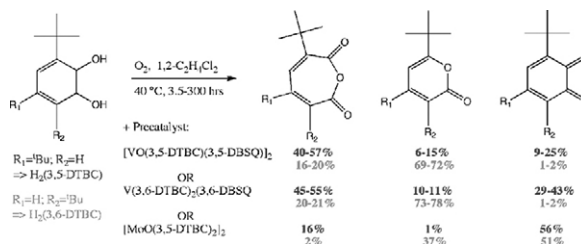
Supported N-heterocyclic carbene rhodium complexes as highly selective hydroformylation catalysts

New rhodium(I) N-heterocyclic carbene complexes supported on polymeric monoliths applied as catalyst precursors of 1-hexene hydroformylation at 10 atm of CO/H<sub>2</sub> with a small amount of P(OPh)<sub>3</sub> as a modifying ligand, produced ca. 80% of aldehydes with n/iso ratio of ca. 6 in eight successive runs.

**Aimee M. Morris, Cortlandt G. Pierpont, Richard G. Finke***Journal of Molecular Catalysis A: Chemical* 309 (2009) 137

Dioxygenase catalysis by d<sup>0</sup> metal-catecholate complexes containing vanadium and molybdenum with H<sub>2</sub>(3,5-DTBC) and H<sub>2</sub>(3,6-DTBC) substrates

The dioxygenase activity of the three precatalysts [VO(3,5-DTBC)(3,5-DBSQ)]<sub>2</sub> (where 3,5-DTBC = 3,5-di-*tert*-butylcatecholate and 3,5-DBSQ = 3,5-di-*tert*-butylsemiquinone), V(3,6-DTBC)<sub>2</sub>(3,6-DBSQ), and [MoO(3,5-DTBC)<sub>2</sub>]<sub>2</sub> was investigated with H<sub>2</sub>(3,5-DTBC) and H<sub>2</sub>(3,6-DTBC) substrates shown below. Interestingly, intradiol and extradiol dioxygenase products are observed for both the H<sub>2</sub>(3,5-DTBC) and H<sub>2</sub>(3,6-DTBC) substrates with the V-precatalysts, while the Mo-precatalyst gives a majority of the less interesting autoxidation product, benzoquinone.



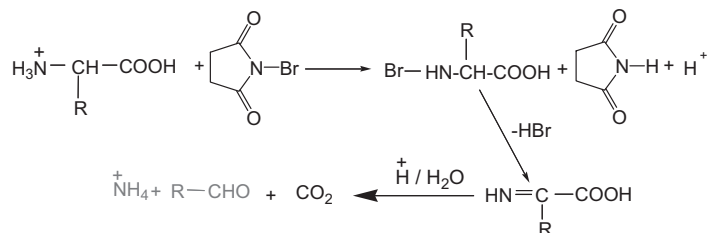


**M.N. Kumara, N.S. Linge Gowda, K. Mantelingu, Kanchugara Koppal S. Rangappa**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 172

*N*-Bromosuccinimide assisted oxidation of tripeptides and their amino acid analogs: Synthesis, kinetics, and product studies

Tripeptides (TPs) namely, glycyl-valyl-glycine (Gly-Val-Gly), alanyl-valyl-glycine (Ala-Val-Gly) and glycyl-phenylalanyl-glycine (Gyl-Phe-Gly) were synthesized by classical solution phase methods and characterized. The kinetics of oxidation of tripeptides (TPs) and their amino acids (AAs) analogs by *N*-bromosuccinimide (NBS) was studied in the presence of perchloric acidic medium at 28 °C. Where R = -H for glycine; R = -CH<sub>3</sub> for alanine; R = -CH(-CH<sub>3</sub>)<sub>2</sub> for valine; R = -CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub> for phenylalanine.

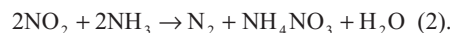
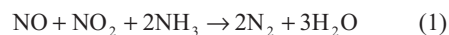


**Md. Azhar Uddin, Koichiro Shimizu, Koji Ishibe, Eiji Sasaoka**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 178

Characteristics of the low temperature SCR of NO<sub>x</sub> with NH<sub>3</sub> over TiO<sub>2</sub>

Low temperature selective catalytic reduction (LT-SCR) of NO + NO<sub>2</sub> mixture with NH<sub>3</sub> was investigated over TiO<sub>2</sub>, SiO<sub>2</sub> and activated carbon at 100 °C under atmospheric pressure. The presence of SO<sub>2</sub> and O<sub>2</sub> was essential for the selective removal of NO with NH<sub>3</sub> over TiO<sub>2</sub>. The presence of SO<sub>2</sub> contributed to the oxidation of NO to NO<sub>2</sub> over TiO<sub>2</sub>. If NO<sub>2</sub> existed with NO in the reaction system, the presence of SO<sub>2</sub> was not necessary for the removal of NO over TiO<sub>2</sub>. The following two reactions were suggested to occur over TiO<sub>2</sub>. The reaction (2) occurred on all three catalysts, however the reaction (1) did not proceed significantly over SiO<sub>2</sub>.



**Guang-Cheng Yang, Xiao-Qing Jia, Ren-Ming Pan, Heng-Dao Quan**

*Journal of Molecular Catalysis A: Chemical* 309 (2009) 184

The disproportionation of CF<sub>2</sub> carbene in vapor-phase pyrolysis reaction over activated carbon and porous aluminum fluoride

The disproportionation of CF<sub>2</sub> carbene in vapor-phase pyrolysis reaction over activated carbon and porous aluminum fluoride.

