



Journal of Molecular Catalysis A: Chemical 278 (2007) v-xiii

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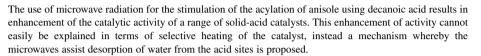
Contents

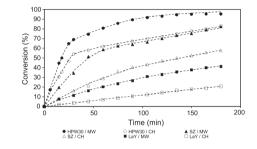
Articles

G. Bond, J.A. Gardner, R.W. McCabe, D.J. Shorrock

Journal of Molecular Catalysis A: Chemical 278 (2007) 1

Friedel-Crafts acylation reactions using heterogeneous catalysts stimulated by conventional and microwave heating



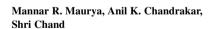


Haiyang Cheng, Jianmin Hao, Hongjun Wang, Chunyu Xi, Xiangchun Meng, Shuxia Cai, Fengyu Zhao A higher ee value of 60.5% has been obtained for enantioselective hydrogenation of acetophenone with a 5 wt.% Ru/γ -Al₂O₃ catalyst modified by *R*,*R*-1,2-diphenylethylene-diamine and phosphine ligand.

(*R*,*R*)-DPEN, TPP KOC(CH₃)₃, solvent

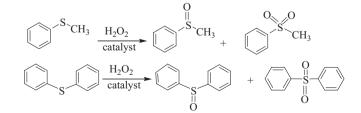
Journal of Molecular Catalysis A: Chemical 278 (2007) 6

(R,R)-DPEN-modified Ru/ γ -Al₂O₃—An efficient heterogeneous catalyst for enantioselective hydrogenation of acetophenone



Journal of Molecular Catalysis A: Chemical 278 (2007) 12

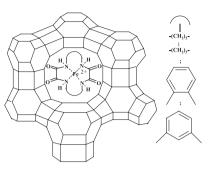
Oxidation of methyl phenyl sulfide, diphenyl sulfide and styrene by oxovanadium(IV) and copper(II) complexes of NS donor ligand encapsulated in zeolite-Y Oxovanadium(IV) and copper(II) complexes of monobasic bidentate NS donor, 2-mercaptomethylbenzimidazole (Htmbmz) have been encapsulated in the cavity of zeolite-Y and characterized. These complexes catalyze the oxidation, by hydrogen peroxide and *tert*-butylhydroperoxide, of styrene, methyl phenyl sulfide and diphenyl sulfide in good yield.



Masoud Salavati-Niasari

Journal of Molecular Catalysis A: Chemical 278 (2007) 22

Synthesis, characterization and catalytic epoxidation of styrene using molecular oxygen over "neat" and host–guest nanocomposite materials $Bzo_2[12]aneN_4$: dibenzo-1,4,7,10-tetraazacyclododecane-2,3,8,9-tetraone and $Bzo_2[14]aneN_4$: dibenzo-1,4,8,11-tetraazacyclotetradecane-2,3,9,10-tetraone. Iron(II) complexes with azamacrocyclic ligand were entrapped in the nanocavity of zeolite-Y by a two-step process in the liquid phase: (i) adsorption of [bis(diamine)iron(II)]; [Fe(N-N)₂]@NaY; in the supercages of the zeolite, and (ii) in situ condensation of the iron(II) precursor complex with diethyloxalate. These new nanocatalyst materials are efficient heterogeneous catalysts for the epoxidation of styrene with molecular oxygen in the absence of a sacrificial reductant.

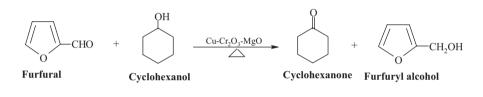


B.M. Nagaraja, A.H. Padmasri, P. Seetharamulu, K. Hari Prasad Reddy, B. David Raju, K.S. Rama Rao

A highly active Cu-MgO-Cr₂O₃ catalyst for simultaneous formation of cyclohexanone and furfuryl alcohol in a novel coupling route from cyclohexanol and furfural is advantageous in terms of avoiding external H_2 supply and the presence of Cu⁰/Cu⁺ species with the smaller Cu particle size at the surface are responsible for good yields.

Journal of Molecular Catalysis A: Chemical 278 (2007) 29

A highly active Cu-MgO- Cr_2O_3 catalyst for simultaneous synthesis of furfuryl alcohol and cyclohexanone by a novel coupling route—Combination of furfural hydrogenation and cyclohexanol dehydrogenation

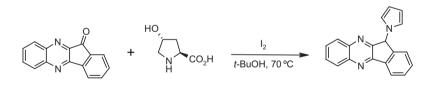


J.S. Yadav, B.V. Subba Reddy, Ruchi Jain, U.V. Subba Reddy

Journal of Molecular Catalysis A: Chemical 278 (2007) 38

Iodine-catalyzed coupling of 4-hydroxyproline with isatins: An expeditious synthesis of 3-pyrrolyl indolin-2-ones

Iodine is found to catalyze efficiently the coupling of 4-hydroxyproline with isatins under mild conditions to produce 3-(1*H*-pyrrol-1-yl)indolin-2-one and 11-(1*H*-pyrrol-1-yl)-11*H*-indeno[1,2-*b*]quinoxalin-11-ones in excellent yields.

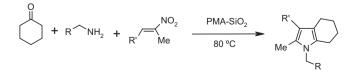


J.S. Yadav, B.V. Subba Reddy, T. Srinivasa Rao, R. Narender, Manoj K. Gupta

A mild and efficient method for the synthesis of highly substituted pyrroles is described using phosphomolybdic acid supported on silica gel as a reusable catalyst. The use of PMA supported on silica gel makes it quite simple, more convenient and environmentally friendly.

Journal of Molecular Catalysis A: Chemical 278 (2007) 42

 PMA/SiO_2 as efficient, cost-effective and recyclable catalytic system for the synthesis of highly substituted pyrroles



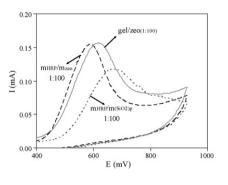
Contents

R.H. Carvalho, F. Lemos, M.A.N.D.A. Lemos, J.M.S. Cabral, F. Ramôa Ribeiro

Journal of Molecular Catalysis A: Chemical 278 (2007) 47

Electro-oxidation of phenol on a new type of zeolite/graphite biocomposite electrode with horseradish peroxidase A novel biocomposite electrode containing horseradish peroxidase (HRP) and zeolite co-immobilized on gelatin particles mixed with graphite was described. Comparing the composite (zeolite/graphite) and the biocomposite (gelatin/HRP/zeolite/graphite) electrodes showed that the latter presented an enhancement on the electrodes diffusion properties and, apparently, the enzyme co-immobilized with zeolite on gelatin was electro-active and functioned as mediator in the electro-oxidation of phenol. Various HRP/zeolite ratios were tested and the best result was obtained with the 1:100 $m_{\rm HRP}/m_{zeo}$ biocomposite electrode. These results confirm the existence of HRP-zeolite interactions, as previously observed in

pseudo-homogeneous oxidation of phenol.



Hussein Hamad, Michel Soulard, Bénédicte Lebeau, Joël Patarin, Tayssir Hamieh, Joumana Toufaily, Hakim Mahzoul

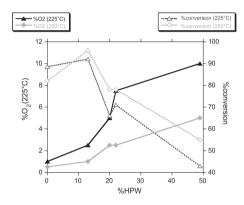
Journal of Molecular Catalysis A: Chemical 278 (2007) 53

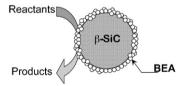
A new way for deNO_x catalyst preparation: Direct incorporation of 12-tungstophosphoric acid $H_3PW_{12}O_{40}$ and platinum into mesoporous molecular sieves material

Gauthier Winé, Zora El Berrichi, Cuong Pham-Huu

Journal of Molecular Catalysis A: Chemical 278 (2007) 64

BETA zeolite supported on silicon carbide for Friedel-Crafts fixed-bed reactions



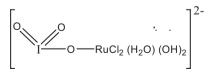


Ashok Kumar Singh, Shalini Srivastava, Jaya Srivastava, Rashmi Srivastava, Priyanka Singh

Journal of Molecular Catalysis A: Chemical 278 (2007) 72

Studies in kinetics and mechanism of oxidation of D-glucose and D-fructose by alkaline solution of potassium iodate in the presence of Ru(III) as homogeneous catalyst

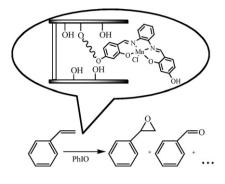
Kinetics of oxidation of D-glucose and D-fructose by alkaline solution of potassium iodate in the presence of Ru(III) as homogeneous catalyst have been studied. Observed kinetic data with spectrophotometric evidence led us to propose that there is a formation of most reactive activated complex, in the rate determining step by the interaction of two different species, i.e. $[RuCl_2(H_2O)_2(OH)_2]^-$ and IO_3^- .



Iwona Kuźniarska-Biernacka, Ana R. Silva, Ana P. Carvalho, João Pires, Cristina Freire

Journal of Molecular Catalysis A: Chemical 278 (2007) 82

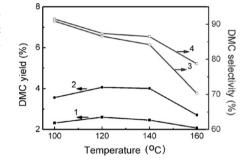
Direct immobilisation *versus* covalent attachment of a Mn(III)*salen* complex onto an Al-pillared clay and influence in the catalytic epoxidation of styrene A Mn(III)salen complex has been directly immobilised and covalently attached onto organo-functionalised pillared clays. The new materials have been characterised and tested in the catalytic epoxidation of styrene with iodosylbenzene as an oxygen source.



X.J. Wang, M. Xiao, S.J. Wang, Y.X. Lu, Y.Z. Meng

Journal of Molecular Catalysis A: Chemical 278 (2007) 92

Direct synthesis of dimethyl carbonate from carbon dioxide and methanol using supported copper (Ni, V, O) catalyst with photo-assistance A copper modified (Ni, V, O) semiconductor complex catalyst was synthesized and utilized in the direct syntheses of DMC from CO_2 and CH_3OH . The results demonstrated that the catalytic activity was enhanced with the assistance of ultraviolet (UV) irradiation compared with the pure thermal and surface catalytic reaction.

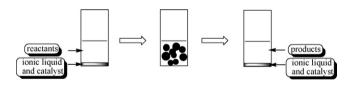


Jia Jian Peng, Jia Yun Li, Ying Bai, Wei Hong Gao, Hua Yu Qiu, Hui Wu, Yuan Deng, Guo Qiao Lai

Journal of Molecular Catalysis A: Chemical 278 (2007) 97

 $\rm Rh(PPh_3)_3Cl/ionic$ liquid (molten salt) as a thermoregulated and recyclable catalytic system for hydrosilylation

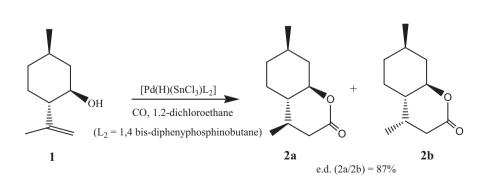
 $Rh(PPh_3)_3$ Cl/ionic liquid (molten salt) used as thermoregulated and recyclable catalytic system for hydrosilylation had been investigated. The hydrosilylation process could be influenced by the alkyl chains attached on the pyridinium and imidazolium cations. And this catalyst system combines the advantages of ionic liquid with convenient product separation.



Lisa Diab, Maryse Gouygou, Eric Manoury, Philippe Kalck, Martine Urrutigoïty

Journal of Molecular Catalysis A: Chemical 278 (2007) 102

Critical solvent effect on the chiral recognition of a catalytic species by a chiral substrate

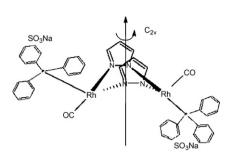


Pablo J. Baricelli, Tirza Ascanio, Eduardo Lujano, Luis G. Melean, Margarita Borusiak, Francisco López-Linares, Luis Jhonatan Bastidas, Merlín Rosales

Journal of Molecular Catalysis A: Chemical 278 (2007) 107

Aqueous biphasic catalytic hydrogenation of olefins and olefin mixtures by the [Rh(u- $Pz)(CO)(TPPMS)]_2$ complex, Pz = pyrazolate, TPPMS = $(C_6H_5)_2\tilde{P}(C_6H_4SO_3Na)$

The complex [Rh((-Pz)(CO)(TPPMS)]2 was used as a catalytic precursor for the aqueous biphasic hydrogenation of several olefins and olefins mixtures resembling naphtha cuts. The observed catalytic activity was 1-hexane > styrene > cyclohexene > 2,3-dimethyl-1-butene. The catalyst was shown to be resistant to sulfur poisons and recyclable for five consecutive runs without loss of activity.

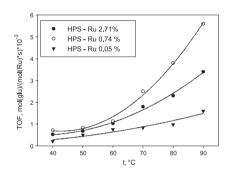


Esther Sulman, Valentine Doluda, Stanislaw Dzwigaj, Eric Marceau, Leonid Kustov, Olga Tkachenko, Alexev Bykov, Valentina Matveeva, Mikhail Sulman, Natalia Lakina

Journal of Molecular Catalysis A: Chemical 278 (2007) 112

Catalytic properties of Ru nanoparticles introduced in a matrix of hypercrosslinked polystyrene toward the low-temperature oxidation of D-glucose

The catalytic properties and structural characterization of catalysts derived from hypercrosslinked polystyrene (HPS), a polymer exhibiting mesoporosity and loaded with ruthenium in various amounts, are investigated in the oxidation of D-glucose to D-gluconic acid. Transmission electron microscopy, X-ray fluorescence analysis, nitrogen physisorption measurements, diffuse reflectance infrared Fourier transform spectroscopy of adsorbed CO, EXAFS, XANES and catalytic studies show the presence of catalytically active nanoparticles of mixed composition (metal/oxide) with a mean diameter of 1-2 nm.

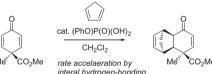


Ryukichi Takagi, Asako Kondo, Katsuo Ohkata

Journal of Molecular Catalysis A: Chemical 278 (2007) 120

Rate acceleration of phosphoric acid-catalyzed Diels-Alder reaction by internal hydrogen-bonding of adjacent hydroxy group

The Brønsted acid-catalyzed Diels-Alder reaction was examined. Phosphoric acids were effective Brønsted acids for the Diels-Alder reaction of cyclohexadienones and activated by the internal hydrogen-bonding of the adjacent hydroxy group.



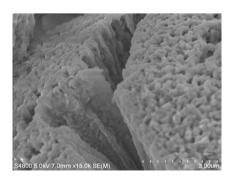
interal hydrogen-bonding

Hanna-Leena Rönkkö, Hilkka Knuuttila, Peter Denifl, Timo Leinonen, Tapani Venäläinen

Journal of Molecular Catalysis A: Chemical 278 (2007) 127

Structural studies on a solid self-supported Ziegler-Natta-type catalyst for propylene polymerization

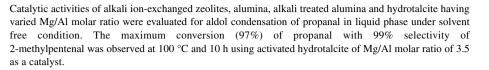
The article describes structural studies on a solid MgCl₂-based TiCl₄ Ziegler-Natta catalyst for propylene polymerization prepared via emulsion technique. Although the surface area of this selfsupported catalyst sample is exceptionally low, the activity is high. SEM measurements revealed an intriguing structure: evidently the catalyst particle is composed of nanoribbons (figure) that extend from the center of the particle to the surface.

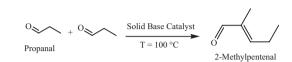


Sumeet K. Sharma, Parimal A. Parikh, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 278 (2007) 135

Solvent free aldol condensation of propanal to 2-methylpentenal using solid base catalysts

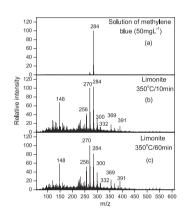




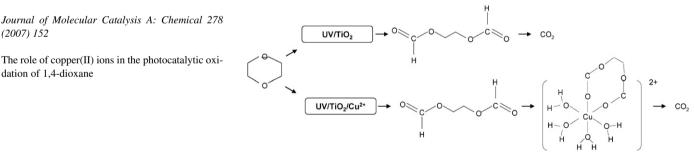
Wladmir F. de Souza, Iara R. Guimarães, Luiz C.A. Oliveira, Mário C. Guerreiro, Aline L.N. Guarieiro, Kele T.G. Carvalho

Journal of Molecular Catalysis A: Chemical 278 (2007) 145

Natural and H_2 -reduced limonite for organic oxidation by a Fenton-like system: Mechanism study via ESI-MS and theoretical calculations In this work the reactivity of the Fenton heterogeneous system $\text{HCOOC//H}_2\text{O}_2$ using thermal treated limonite was studied. Experiments were carried out to investigate the effect of formic acid contents and Fe^{2+} sites in iron oxide applied to the methylene blue dye oxidation, using a Fenton-like heterogeneous and intermediates formation monitored by ESI-MS.



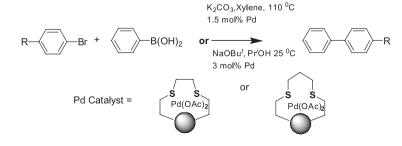
S.W. Lam, M. Hermawan, H.M. Coleman, K. Fisher, R. Amal



Mohammed Al-Hashimi, Asma Qazi, Alice C. Sullivan, John R.H. Wilson

Journal of Molecular Catalysis A: Chemical 278 (2007) 160

Dithio palladium modified silicas—New heterogeneous catalysts for Suzuki cross-coupling reactions In this paper we report on new silica immobilized di(ethylthio)ethane and di(ethylthio)propane palladium catalysts where the presence of two sulfur donor atoms in the immobilized ligands assist Pd binding. Catalyst synthesis and use in Suzuki coupling chemistry under two different sets of conditions, isopropanol at room temperature and hot xylene is reported. The catalysts may be recycled and are resistant to leaching in both cases.

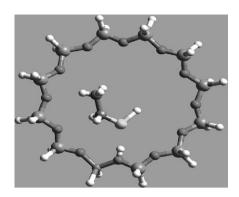


Humberto Soscún, Olga Castellano, Javier Hernandez, Federico Arrieta, Yaneth Bermúdez, Alan Hinchliffe, Marcos Rosa Brussin, Morella Sanchez, Anibal Sierraalta, Fernando Ruette

Journal of Molecular Catalysis A: Chemical 278 (2007) 165

An ab initio and DFT study of the interaction between ethanethiol and zeolites

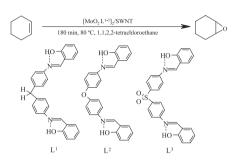
The manuscript reports the first theoretical investigation about the interaction of ethanethiol with an acid zeolite as represented for a cluster of 12-membered ring that has been fully optimized with Hartree–Fock and B3LYP methods at C_s symmetry. The results leads to the formation of an etanethiol–zeolite complex which properties are similars to previous reported that represent the adsorption of sulfur compounds in acid zeolites. The calculations consist of structural, electronic, energetic and vibrational aspects of the sulfur compound–zeolites complexes.



Masoud Salavati-Niasari, Mehdi Bazarganipour

Journal of Molecular Catalysis A: Chemical 278 (2007) 173

Effect of single-wall carbon nanotubes on direct epoxidation of cyclohexene catalyzed by new derivatives of *cis*-dioxomolybdenum(VI) complexes with bis-bidentate Schiff-base containing aromatic nitrogen–nitrogen linkers The synthesis and characterisation of three dimeric *cis*-dioxomolybdenum(VI) complexes involving Schiff-base ligands is described. Ligands were obtained by condensation of salicylaldehyde with aromatic nitrogen–nitrogen linkers. [MoO₂(acac)₂] reacted with the prepared ligands forming six-coordinated *cis*-dioxoMo(VI) complexes; [MoO₂L^{1–3}]₂. These complexes show good catalytic activity and selectivity in the epoxidation of cyclohexene with *t*-butylhydroperoxide (TBHP), especially for complex [MoO₂L³]₂, which could give a nearly 88% of epoxidation conversion and 94% of selectivity. The addition of single-wall carbon nanotubes (SWNT) can enhance the conversion of the Mo complexes and the selectivity of epoxide.



Beatriz de Rivas, Rubén López-Fonseca, Juan R. González-Velasco, José I. Gutiérrez-Ortiz

Journal of Molecular Catalysis A: Chemical 278 (2007) 181

On the mechanism of the catalytic destruction of 1,2-dichloroethane over Ce/Zr mixed oxide catalysts

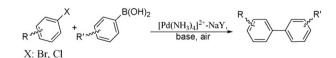
The oxidation mechanism of the oxidation of 1,2-dichloroethane on Ce/Zr mixed oxides was investigated by means of a combined flow and infrared spectroscopy study. The decomposition occurs through by dehydrochlorination into vinyl chloride in the presence of acid sites. This intermediate can be attacked by nucleophilic oxygen species from the catalyst to form chlorinated alkoxide species, which readily decompose to gradually generate acetaldehyde, acetates and CO_x .

$$\begin{array}{c} CH_2CI-CH_2CI \xrightarrow{-HCI}_{Lewis} + CH_2=CHCI \xrightarrow{H^+}_{Humidity} CH_3^+CHCI \\ \xrightarrow{IOI}_{Sites} + CH_3^+C_1^+C_1^+ + HCI \\ \xrightarrow{IOI}_{H_3} + CH_3^+C_1^+C_1^+ + CO_x^+ + H_2O \\ \xrightarrow{IOI}_{H_3} + CO_x^+ + CO_x^+$$

Gülay Durgun, Özge Aksın, Levent Artok

Journal of Molecular Catalysis A: Chemical 278 (2007) 189

Pd-loaded NaY zeolite as a highly active catalyst for ligandless Suzuki–Miyaura reactions of aryl halides at low Pd loadings under aerobic conditions Palladium-loaded NaY zeolite was found to be a highly active catalyst precursor for Suzuki–Miyaura (SM) reactions of aryl bromides and aryl chlorides at low Pd concentrations in air. The presence of excess amounts of moist zeolite promoted the reactions of aryl chlorides.

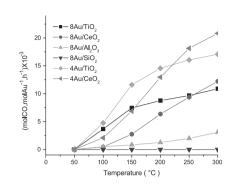


Alberto Sandoval, Antonio Gómez-Cortés, Rodolfo Zanella, Gabriela Díaz, José M. Saniger

Journal of Molecular Catalysis A: Chemical 278 (2007) 200

Gold nanoparticles: Support effects for the WGS reaction

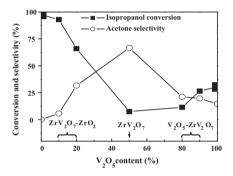
Gold nanoparticles supported on reducible and nonreducible oxides with comparable gold particle size were studied in the WGS reaction. The activity of Au on reducible oxides was much higher than the one observed on non-reducible oxides. The optimum calcination temperature was 300 °C. For samples calcined at 300 °C and reaction temperatures below 225 °C the activity varied as follows: TiO₂ > CeO₂ ≫ Al₂O₃ ≫ SiO₂



Jiazhen Ge, Mingwei Xue, Qing Sun, Aline Auroux, Jianyi Shen

Journal of Molecular Catalysis A: Chemical 278 (2007) 209

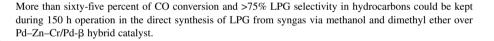
Surface acidic and redox properties of V-Zr-O catalysts for the selective oxidation of toluene to benzaldehyde A series of V-Zr-O (V_2O_5 -ZrO_2) complex oxides were prepared by the sol-gel method, and ZrV_2O_7 was found to be the main phase in the 50% V_2O_5 -ZrO₂, which exhibited the significantly lower surface acidity and relatively stronger redox ability as evidenced by the probe reaction of isopropanol conversion in air, and thus, the better reactivity for the selective oxidation of toluene to benzaldehyde and benzoic acid.

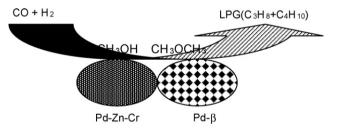


Qingjie Ge, Xiaohong Li, Hiroshi Kaneko, Kaoru Fujimoto

Journal of Molecular Catalysis A: Chemical 278 (2007) 215

Direct synthesis of LPG from synthesis gas over Pd–Zn–Cr/Pd- β hybrid catalysts

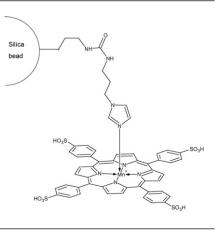




Paolo Zucca, Giuseppe Mocci, Antonio Rescigno, Enrico Sanjust

Journal of Molecular Catalysis A: Chemical 278 (2007) 220

5,10,15,20-Tetrakis(4-sulfonato-phenyl)porphine-Mn(III) immobilized on imidazole-activated silica as a novel lignin-peroxidase-like biomimetic catalyst A new biomimetic lignin-peroxidase-like heterogeneous catalyst was investigated. It could be of potential interest for oxidative degradation of plant effluents, containing soluble lignin derivatives. 5,10,15,20-Tetrakis(4-sulfonato-phenyl)porphine-Mn(III) was coordinated to imidazole-bearing silica to give a stable adduct. This showed a remarkable ability to catalyze veratryl alcohol oxidation at the expenses of H_2O_2 . Kinetic and operational characterisation of the catalyst is also reported.



Z.S. Liu, G.L. Rempel

Journal of Molecular Catalysis A: Chemical 278 (2007) 228

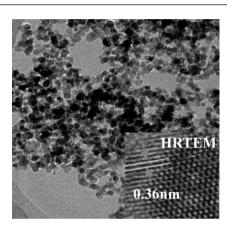
The triphasic transfer hydrogenation of aromatic aldehydes by aqueous sodium formate in the presence of heterogenized ruthenium(II) complexes bound to swellable polymer matrices Aromatic aldehydes can be reduced to the corresponding alcohols by hydrogen transfer from HCO_2Na in the presence of Ru(II) complexes bound to swellable polymer matrices and a quaternary ammonium salt. The reaction kinetics have been measured between 50 and 80 °C. The process was shown to depend on the structure of the aldehyde acceptor, on the concentrations of formate donor and phase-transfer agent, on the amount of the catalyst and also to be sensitive to the polarity of the organic solvent. The observed activation energy, $E_a = 20.80$ kcal mol⁻¹, suggests that process is a predominantly chemically controlled reaction. A general reaction mechanism and rate equation have been proposed.

ArCHO_(org) + HCOONa_(aq) + H₂O
$$\xrightarrow{Q^+Z^-}$$
 ArCH₂OH_(org) + NaHCO₃(aq)

Yuning Huo, Jian Zhu, Jingxia Li, Guisheng Li, Hexing Li

Journal of Molecular Catalysis A: Chemical 278 (2007) 237

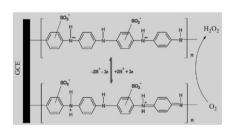
An active La/TiO₂ photocatalyst prepared by ultrasonication-assisted sol-gel method followed by treatment under supercritical conditions A novel La-doped TiO_2 nanocrystals have been successful prepared via a supercritical drying method combined with ultrasonic treatment. The promoting effects of ultrasonication, supercritical treatment, and La-modification are discussed by considering the enhanced particle dispersion, the higher crystallization degree of anatase and the increase of the surface oxygen vacancies and/or defects.



S. Ashok Kumar, Shen-Ming Chen

Journal of Molecular Catalysis A: Chemical 278 (2007) 244

Electrocatalytic reduction of oxygen and hydrogen peroxide at poly(*p*-aminobenzene sulfonic acid)modified glassy carbon electrodes The electrocatalytic ability of the modified electrodes for the reduction of dioxygen to hydrogen peroxide was investigated by using cyclic voltammetry and chronocoulometry techniques at poly(p-aminobenzene sulfonic acid) (PABS)-modified glassy carbon electrodes. For the first time, the electrochemical reduction of oxygen (O₂) has been studied on PABS-modified glassy carbon electrode in pH 7.0 buffer solution using the rotating ring disk electrode (RRDE). In addition, we tested amperometric determination of hydrogen peroxide by using PABS modified GC electrode. In addition, we tested amperometric determination of hydrogen peroxide by using PABS modified GC electrode.



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CO-ethene copolymerisation catalysed by [PdCl₂(PPh₃)₂]/PPh₃/HCl in MeOH

 $[PdCl_2(PPh_3)_2]/PPh_3/HCl$ catalyses the carbonylation of ethene in MeOH to give methyl propanoate and/or a polyketone. The catalytic system is active only in the presence of HCl and is stable up to 110 °C when P/Pd is >6/1. At 100 °C, with Pd/P/HCl = 1/6/1600, under 6.0 MPa total pressure, the main product is MP at 1.0 MPa of ethene, whereas is PK when the pressure of the olefin is higher than 4.0 MPa.

