



## Contents

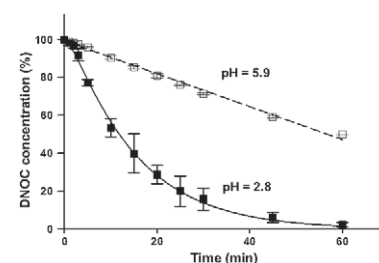
### Articles

**Xia Zeng, Khalil Hanna, Ann T. Lemley**

*Journal of Molecular Catalysis A: Chemical 339 (2011) 1*

Cathodic Fenton degradation of 4,6-dinitro-*o*-cresol with nano-magnetite

► We successfully removed DNOC using nano-magnetite and cathodic Fenton. ► We optimized the electrolyte concentration, electric current, and O<sub>2</sub> flow. ► Homogeneous reaction dominates at low pH and direct electrolysis occurs at neutral. ► Heterogeneous reaction was not obvious under the experimental conditions. ► We developed a model to describe the degradation mechanism at low pH.

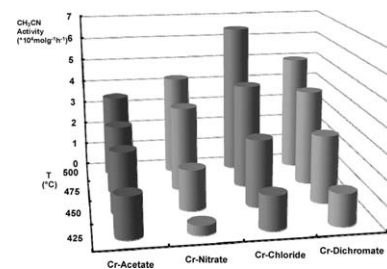


**F. Ayari, M. Mhamdi, D.P. Debecker, E.M. Gaigneaux, J. Alvarez-Rodriguez, A. Guerrero-Ruiz, G. Delahay, A. Ghorbel**

*Journal of Molecular Catalysis A: Chemical 339 (2011) 8*

Effect of the chromium precursor nature on the physicochemical and catalytic properties of Cr–ZSM-5 catalysts: Application to the ammoxidation of ethylene

► Cr–ZSM-5 solids were tested in the ammoxidation of ethylene to acetonitrile. ► There is no destruction of the parent zeolite during solid-state reaction. ► Cr(VI) ions and Cr(III) oxide species are predominant. ► Catalysts are active and selective towards acetonitrile. ► Cr(VI) species are requested in the ammoxidation, while Cr<sub>2</sub>O<sub>3</sub> clusters are inadequate.

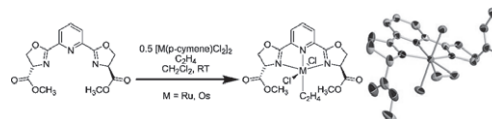


**Kenneth J.H. Young, Kapil S. Lokare, Chin Hin Leung, Mu-Jeng Cheng, Robert J. Nielsen, Nicos A. Petasis, William A. Goddard III, Roy A. Periana**

*Journal of Molecular Catalysis A: Chemical 339 (2011) 17*

Synthesis of osmium and ruthenium complexes bearing dimethyl (*S,S*)-2,2'-(pyridine-2,6-diyl)-bis-(4,5-dihydrooxazol-4-carboxylate) ligand and application to catalytic H/D exchange

► Several new complexes, M(PyBox)Cl<sub>2</sub>(C<sub>2</sub>H<sub>4</sub>), where M = Ru, Os are prepared. ► The Os(PyBox)Cl<sub>2</sub>(C<sub>2</sub>H<sub>4</sub>) complex was characterized by X-ray diffraction. ► All complexes are thermally stable. ► These PyBox compounds are active for C–H activation of benzene.



**Kula Kamal Senapati, Chandan Borgohain, Prodeep Phukan**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 24

Synthesis of highly stable  $\text{CoFe}_2\text{O}_4$  nanoparticles and their use as magnetically separable catalyst for Knoevenagel reaction in aqueous medium

►  $\text{CoFe}_2\text{O}_4$  nanoparticles synthesized without any surfactant or organic capping agent. ► Nanoparticles as well as its dispersion are quite stable. ► Nanoparticles can be used directly as a catalyst without any further modification. ►  $\text{CoFe}_2\text{O}_4$  nanoparticles having basic character can catalyze Knoevenagel reaction. ► The nanocatalyst can be compartmented using an external magnet for reuse.

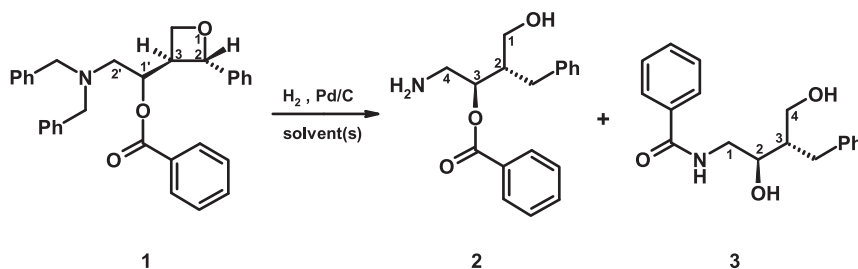


**Ervin Kovács, Angelika Thurner, Ferenc Farkas, Ferenc Faigl, László Hegedűs**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 32

Hydrogenolysis of *N*-protected aminooxetanes over palladium: An efficient method for a one-step ring opening and debenzyl reaction

► One-step hydrogenolysis of an *N*-benzylated aminooxetane derivative. ► Chiral 1,4-aminoalcohol was achieved over a Pd/C catalyst (Selcat Q). ► The selectivity and the yield of the hydrogenation were improved by solvents. ► The best result was obtained in a dichloromethane/methanol solvent mixture (7:3).

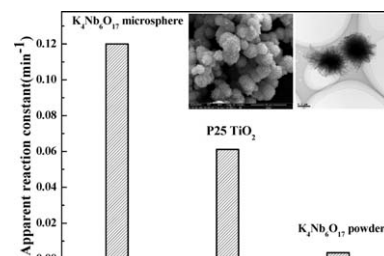


**Chao Zhou, Gang Chen, Qun Wang**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 37

High photocatalytic activity of porous  $\text{K}_4\text{Nb}_6\text{O}_{17}$  microsphere with large surface area prepared by homogeneous precipitation using urea

►  $\text{K}_4\text{Nb}_6\text{O}_{17}$  microsphere with large surface area was synthesized for the first time. ► Higher photodegradation efficiency, two times higher than that of the Degussa P25. ► High photocatalytic activity for water splitting into  $\text{H}_2$  with a rate of 3.0 mmol/h. ► New strategy for design of photocatalysts with large surface areas and high activity.

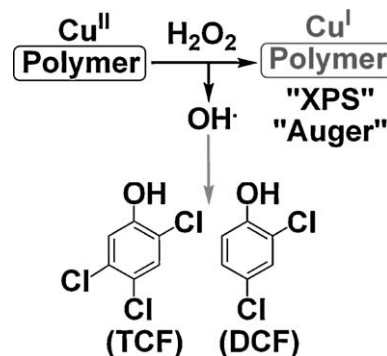


**Juan Manuel Lázaro Martínez, Enrique Rodríguez-Castellón, Rosa María Torres Sánchez, Lisandro Roberto Denaday, Graciela Yolanda Buldain, Viviana Campo Dall'Orto**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 43

XPS studies on the  $\text{Cu(I,II)}$ -polyampholyte heterogeneous catalyst: An insight into its structure and mechanism

►  $\text{Cu(II)}$ -polymer catalyst was applied in the oxidation of chlorinated phenols. ►  $\text{Cu(I)}$  was proved to be an intermediary specie by Auger experiments. ► The conversion of  $\text{L-Cu}^+$  to  $\text{L-Cu}^{2+}$  was the slowest step in the catalytic cycle.

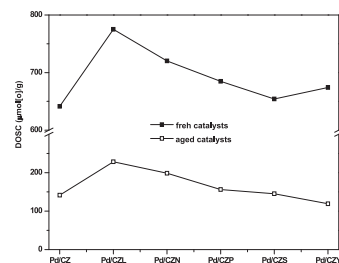


**Qiuyan Wang, Guangfeng Li, Bo Zhao, Renxian Zhou**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 52

The effect of rare earth modification on ceria-zirconia solid solution and its application in Pd-only three-way catalyst

► The effect of rare earth doping on  $\text{Ce}_{0.2}\text{Zr}_{0.8}\text{O}_2$  solid solution is investigated. ► The doping effect on the supported Pd-only three-way catalyst is also studied. ► The addition of La, Nd and Pr results in improved textural/structural properties. ► The addition of La, Nd and Pr leads to improved three-way catalytic performance.

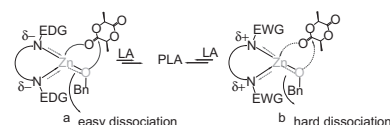


**Hsuan-Ying Chen, Ya-Liu Peng, Tai-Hsiung Huang, Alekha Kumar Sutar, Stephen A. Miller, Chu-Chieh Lin**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 61

Comparative study of lactide polymerization by zinc alkoxide complexes with a  $\beta$ -diketiminato ligand bearing different substituents

► The  $\beta$ -diketiminato zinc alkoxide complexes have been synthesized. ► Their reactivity for the ring-opening polymerization (ROP) of lactide has been studied. ► The electron withdrawing substituents have an inclination to become dinuclear forms. ► The rate of polymerization order: alkyl group  $\sim$  alkoxy  $>$  halide group  $>$  nitro group.

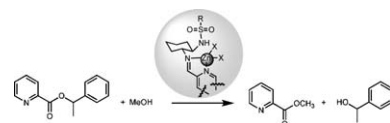


**Ramu Kannappan, Masaomi Matsumoto, John Hallren, Kenneth M. Nicholas**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 72

New chiral Schiff base-zinc complexes and their esterolytic catalytic activity

► New zinc-Schiff base complexes of cyclohexyldiamine-sulfonamides are prepared ► Their ester methanolysis activity for depends on the imine, counteranion and sulfonamide units ► The mechanism is probed via ligand deprotonation and TSA binding experiments.

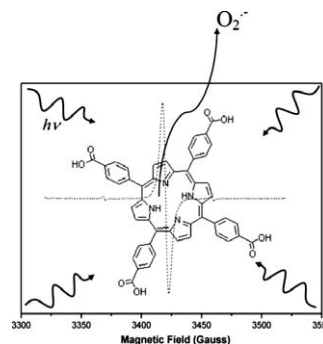


**Gilma Granados-Oliveros, Edgar Alberto Páez-Mozo, Fernando Martínez Ortega, Marilene Turini Piccinato, Fausto Neves Silva, Carmen Luísa Barbosa Guedes, Eduardo Di Mauro, Marcello Ferreira da Costa, André Tsutomu Ota**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 79

Visible light production of superoxide anion with MCarboxyphenylporphyrins (M = H, Fe, Co, Ni, Cu, and Zn) free and anchored on  $\text{TiO}_2$ : EPR characterization

► EPR signals are produced by unpaired electrons on oxygen and porphyrin  $\pi$ -system. ► TcPPM anchored on  $\text{TiO}_2$  show 300 times less intense signal than the free porphyrins. ► Free TcPPZn and TcPPH show highest photoactivity. ► TcPPCu on  $\text{TiO}$  showed the highest photoactivity.

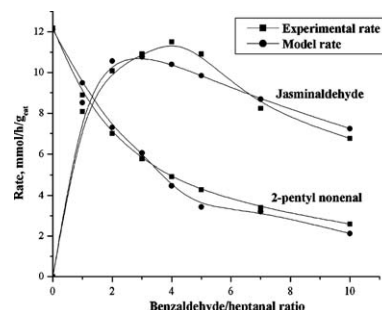


**N. Sudheesh, Sumeet K. Sharma,  
Munir D. Khokhar, Ram S. Shukla**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 86

Kinetic investigations on the modified chitosan catalyzed solvent-free synthesis of jasminaldehyde

► Kinetics on the synthesis of jasminaldehyde over modified chitosan as a catalyst. ► Initial first order followed by saturation kinetics for the amount of catalyst. ► A critical amount of heptanal was needed for the formation of jasminaldehyde. ► The kinetics follows best fit with Langmuir–Hinshelwood rate model.

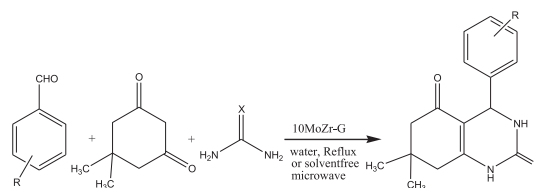


**Satish Samantaray, B.G. Mishra**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 92

Combustion synthesis, characterization and catalytic application of MoO<sub>3</sub>-ZrO<sub>2</sub> nanocomposite oxide towards one pot synthesis of octahydroquinazolinones

► MoO<sub>3</sub>-ZrO<sub>2</sub> nanocomposite was synthesized by combustion method using glycine as fuel. ► Selective stabilization of tetragonal phase of zirconia was observed. ► Presence of well dispersed MoO<sub>3</sub> in the form of isolated and cluster molybdates. ► The particle size of the nanocomposites is in the range of 5–40 nm. ► MoO<sub>3</sub>-ZrO<sub>2</sub> oxide highly efficient catalyst for synthesis of octahydroquinazolinones.

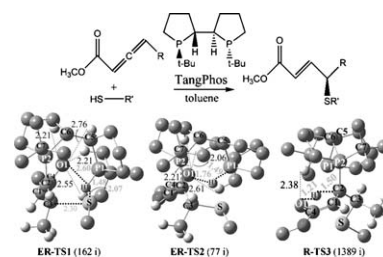


**Nan Lu, Lin Meng, Dezhan Chen, Guiqiu Zhang**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 99

Theoretical mechanistic study of TangPhos-catalyzed asymmetric  $\gamma$  addition of thiols to allenates

► This is the first theoretical study on TangPhos-catalyzed asymmetric  $\gamma$  addition. ► Reaction involves nucleophilic attack of S to  $\gamma$ -carbon and two times proton transfer. ► Bond  $\beta$ -carbon – P2 shifts positive charge of C2 leaving C3 as electrophilic center. ► P1 abstracts proton of thiol and facilitates proton transfer as a shuttle. ► Enantioselectivity is exerted by rigid chiral rings and bulky *t*-butyl of TangPhos.

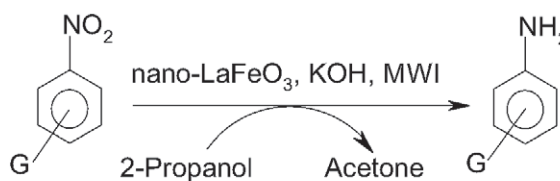


**Saeid Farhadi, Firouzeh Siadatnasab**

*Journal of Molecular Catalysis A: Chemical* 339 (2011) 108

Perovskite-type LaFeO<sub>3</sub> nanoparticles prepared by thermal decomposition of the La[Fe(CN)<sub>6</sub>]-5H<sub>2</sub>O complex: A new reusable catalyst for rapid and efficient reduction of aromatic nitro compounds to arylamines with propan-2-ol under microwave irradiation

► LaFeO<sub>3</sub> nanoparticles were prepared via decomposition of the La[Fe(CN)<sub>6</sub>]-5H<sub>2</sub>O. ► Nitroarenes were reduced to arylamines by propan-2-ol over nano-LaFeO<sub>3</sub> under MWI. ► This method is compatible with other reducible sensitive functionalities. ► The activity of LaFeO<sub>3</sub> nanoparticles is higher than bulk LaFeO<sub>3</sub> sample.



G = various electron donating/withdrawing groups