



## Contents

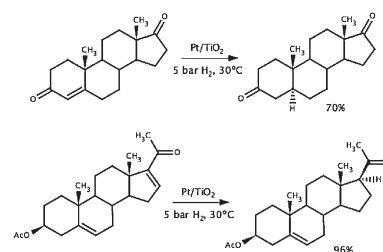
### Articles

**Rui M.D. Nunes, Bruno F. Machado, Mariette M. Pereira, Maria José S.M. Moreno, Joaquim L. Faria**

*Journal of Molecular Catalysis A: Chemical 333 (2010) 1*

Platinum supported on TiO<sub>2</sub> as a new selective catalyst on heterogeneous hydrogenation of  $\alpha,\beta$ -unsaturated oxosteroids

► Pt nanoparticles (4–5 nm) are supported over TiO<sub>2</sub> by photochemical deposition ► Pt/TiO<sub>2</sub> is an efficient catalyst for the hydrogenation of  $\alpha,\beta$ -unsaturated oxosteroids ► The activity and selectivity of these catalysts are pressure independent but the regioselectivity can be modulated by temperature ► The  $\alpha$ -diastereoselectivity was outstanding, comparable to the homogeneous process ► No decrease of activity or selectivity is observed after using the catalyst in 5 consecutive cycles.

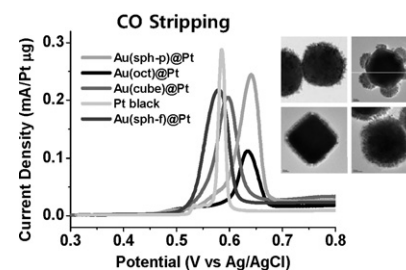


**Minkyu Min, Cheonghee Kim, Hyunjoo Lee**

*Journal of Molecular Catalysis A: Chemical 333 (2010) 6*

Electrocatalytic properties of platinum overgrown on various shapes of gold nanocrystals

► Platinum overgrown on various shapes of gold nanocrystal (cubes, octahedra, spheres) was used as electrocatalysts. ► CO stripping, methanol oxidation, formic acid oxidation, and oxygen reduction reaction were performed on various Au@Pt nanoparticles and Pt black. ► Especially, Au(oct)@Pt nanoparticles showed enhanced specific activity for formic acid oxidation and oxygen reduction reaction.

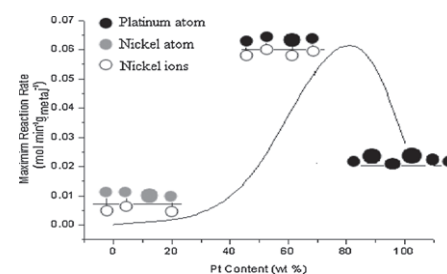


**N.H.H. Abu Bakar, M.M. Bettahar, M. Abu Bakar, S. Monteverdi, J. Ismail**

*Journal of Molecular Catalysis A: Chemical 333 (2010) 11*

Low temperature activation of Pt/Ni supported MCM-41 catalysts for hydrogenation of benzene

► Catalysts containing Pt and Ni as the active phases can be prepared via classical methods and still show optimum activity at low temperatures. The activation temperature employed in this work is only at 473 K for duration of 15 min. This is unusual for Ni based catalysts. A variety of characterization techniques were used to understand this phenomenon. Findings reveal two possible explanations for the enhanced catalytic activity and optimum activity at low activation temperatures: (i) alloying of the Pt/Ni metal phases or/and; (ii) anchoring of the Pt particles to Ni<sup>2+</sup> ions attached to the support. ► Alloying of Pt and Ni is a common occurrence which can contribute to the enhanced reactivity. However, anchoring of the Pt particles to Ni ions is also an important aspect.

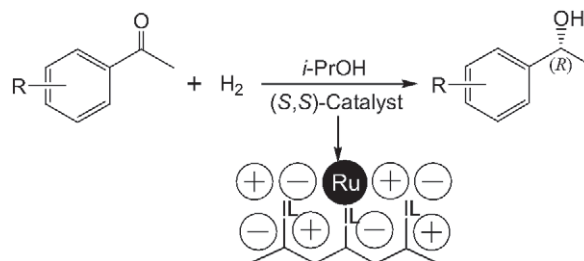


**Lan-Lan Lou, Yanling Dong, Kai Yu, Shu Jiang, Yang Song, Song Cao, Shuangxi Liu**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 20

Chiral Ru complex immobilized on mesoporous materials by ionic liquids as heterogeneous catalysts for hydrogenation of aromatic ketones

► Chiral Ru complex was immobilized on mesoporous materials by ionic liquids. ► Immobilized catalysts showed as high catalytic performance as homogeneous one. ► Immobilized catalysts were stable and could be easily recovered for reuse. ► Both the two ionic liquids contributed to the high stability of immobilized catalyst.

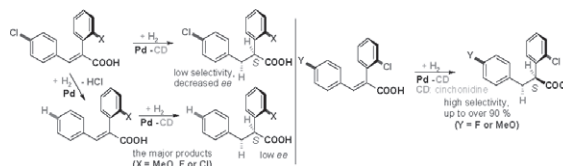


**György Szöllösi, Beáta Hermán, Erika Szabados, Ferenc Fülöp, Mihály Bartók**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 28

Reactions of chlorine substituted (*E*)-2,3-diphenylpropenoic acids over cinchonidine-modified Pd: Enantioselective hydrogenation versus hydrodechlorination

► The enantioselective hydrogenation/hydrogenolysis of Cl substituted (*E*)-2,3-diphenylpropenoic acids over Pd-cinchonidine catalyst was studied. ► The fast hydrodechlorination of the  $\beta$ -phenyl-*para*-Cl was in contrast with the almost exclusive hydrogenation of acids having the Cl on the  $\alpha$ -phenyl ring. ► These were interpreted by the tilted and parallel arrangements of the  $\alpha$ - and  $\beta$ -phenyl rings on the surface. ► The conclusions were used for the rational design of an acid affording up to 95% ee at 295 K.

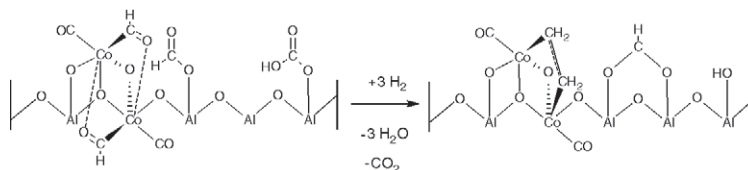


**Márton Kollár, Adriana De Stefanis, Hanna E. Solt, Magdolna R. Mihályi, József Valyon, Anthony A.G. Tomlinson**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 37

The mechanism of the Fischer–Tropsch reaction over supported cobalt catalysts

► Early stages of Fischer–Tropsch synthesis (FTS) do not involve surface carbide species. ► Surface species from FTS are bonded Co–carbonyls, hydrocarbons, and oxygenates. ► H–C=O bridges over [Co- $\mu$ O<sub>2</sub>-Co] units are transition states of FTS.

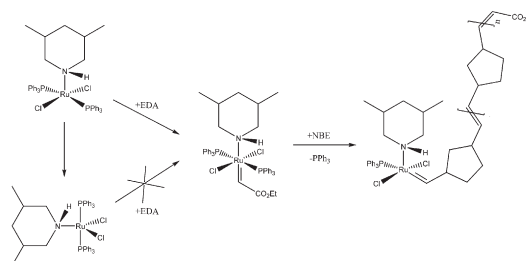


**Valdemiro P. Carvalho Jr., Camila P. Ferraz, Benedito S. Lima-Neto**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 46

Electronic synergism in [RuCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>(amine)] complexes differing the reactivity for ROMP of norbornene and norbornadiene

► Amines as ancillary ligands afforded successful ROMP of NBE and NBD. ► The amines provide different induction period for the Ru–carbene formation. ► The amine  $\sigma \rightarrow \text{Ru} \pi \rightarrow$  monomer electronic synergism is the reason for catalyst efficiency.

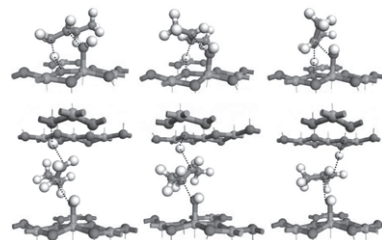


**Hossein A. Dabbagh, Mehdi Zamani, Burtron H. Davis**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 54

Nanoscale surface study and reactions mechanism of 2-butanol over the  $\gamma$ -alumina (1 0 0) surface and nanochannel: A DFT study

► Mechanism of adsorption, dissociation, hydrogen-shift, dehydration and dehydrogenation of adsorbed (*R*)- and (*S*)-2-butanol over the dehydroxylated (1 0 0) surface and nanochannel of  $\gamma$ -alumina defect spinel structure. ► Density functional theory (DFT). ► Asymmetric property of dehydroxylated (1 0 0) surface and nanochannel of  $\gamma$ -alumina defect spinel structure. ► Conformational analysis of adsorbed (*R*)- and (*S*)-2-butanol over the dehydroxylated (1 0 0) surface and nanochannel of  $\gamma$ -alumina defect spinel structure. ► Computation of Mulliken atomic charges of selected basic sites.

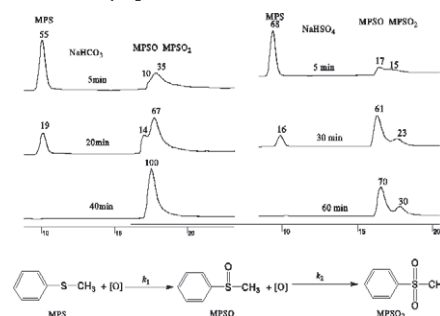


**Hossein Fakhraian, Fardin Valizadeh**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 69

Activation of hydrogen peroxide via bicarbonate, sulfate, phosphate and urea in the oxidation of methyl phenyl sulfide

► In the presence of excess amounts of  $H_2O_2$  and bicarbonate,  $k_1 \sim k_2$ ; separation of the two oxidation steps was impossible; and methyl phenyl sulfone was the sole final oxidation product. ► In the presence of excess amounts of urea, dihydrogen phosphate and hydrogen sulphate,  $k_1 > k_2$ . ► In these cases, separation of the two steps was possible, and by controlling the reaction time, each oxidation product (sulfoxide or sulfone) was obtained.

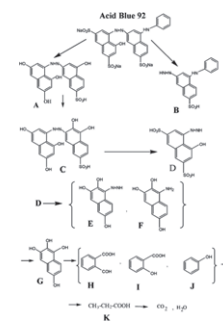


**M. Fathinia, A.R. Khataee, M. Zarei, S. Aber**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 73

Comparative photocatalytic degradation of two dyes on immobilized  $TiO_2$  nanoparticles: Effect of dye molecular structure and response surface approach

► Immobilization of  $TiO_2$  nanoparticles on the glass plates by sol-gel dip-coating method. ► Comparative photocatalytic degradation of an anionic and a cationic dye. ► Optimization of UV/ $TiO_2$  process by central composite design. ► Proposal of photodegradation pathway based on the GC-Mass analysis.

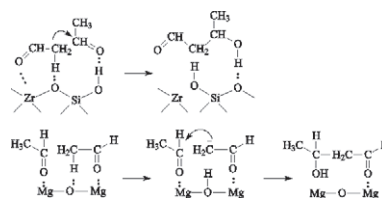


**V.V. Ordonsky, V.L. Sushkevich, I.I. Ivanova**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 85

Study of acetaldehyde condensation chemistry over magnesia and zirconia supported on silica

► Lewis sites and silanols take part in condensation of acetaldehyde over  $ZrO_2/SiO_2$ . ► Two mechanistic pathways operate over  $MgO/SiO_2$ : acidic and basic reaction pathways. ► The key role of Lewis acidic sites in condensation over supported catalysts was shown.

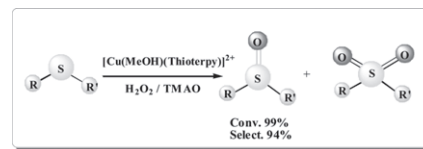


**Ali Nemati Kharat, Abolghasem Bakhoda, Taraneh Hajiashrafi**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 94

Catalytic oxidation of organosulfides to sulfoxides using two novel Cu(II) and Ni(II) complexes with aqueous H<sub>2</sub>O<sub>2</sub>; Effect of TMAO promoter on oxidation of organosulfides

Crystal structures of two new copper(II) and nickel(II) complexes were determined. These complexes were shown catalytic activity for sulfoxidation of a variety of organosulfide substrates.

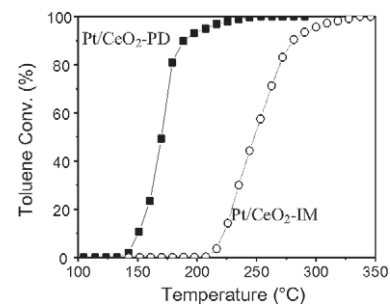


**S. Scirè, C. Crisafulli, S. Giuffrida, G. Ventimiglia, C. Bongiorno, C. Spinella**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 100

Preparation of ceria and titania supported Pt catalysts through liquid phase photo-deposition

► LPPD represents a reliable method for the preparation of supported Pt catalysts. ► Possibility to work at room temperature with simple and low cost equipments. ► LPPD catalysts exhibited homogeneous and very narrow Pt size distribution. ► LPPD catalysts were more active than impregnated ones in the VOC combustion. ► Pt distribution was appropriate for the VOC combustion.

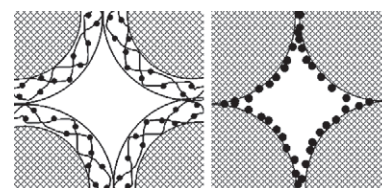


**Karel Jeřábek, Libuše Hanková, Ladislav Holub**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 109

Working-state morphologies of ion exchange catalysts and their influence on reaction kinetics

► Ion exchangers are effective catalysts of fatty acid esterification. ► Their activity depends on alcohol concentration in the reaction mixture. ► Lowering of alcohol concentration inhibits activity of the gel-type catalysts. ► In macroreticular types it promotes access of fatty acid molecules to the acidic centers.

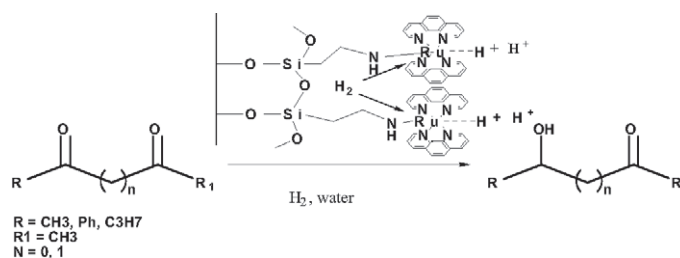


**Amit Deshmukh, Anil Kinage, Rajiv Kumar, Reinout Meijboom**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 114

Heterogenized Ru(II) phenanthroline complex for chemoselective hydrogenation of diketones under biphasic aqueous medium

► Chemoselective hydrogenation of Diketone. ► Utilization of nitrogen containing ligand for the diketone hydrogenation. ► Use of water as reaction medium.

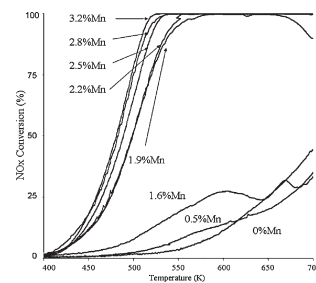


**B. Greenhalgh, M. Fee, A. Dobri, J. Moir, R. Burich, J.-P. Charland, M. Stanciulescu**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 121

DeNO<sub>x</sub> activity–TPD correlations of NH<sub>3</sub>-SCR catalysts

► NH<sub>3</sub>-SCR activity of Mn–CBV zeolite catalyst activity plateaus with metal loading. ► NH<sub>3</sub>-SCR activity correlates with catalyst activity. ► Low temperature activity appears correlated to Lewis acidity associated with metal loading. ► High temperature activity may be correlated to Brønsted acidity.

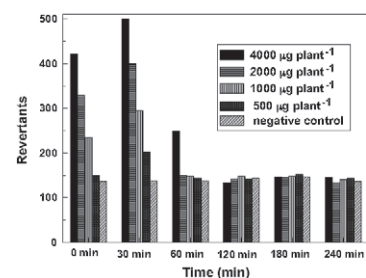


**Taicheng An, Lei Sun, Guiying Li, Shungang Wan**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 128

Gas-phase photocatalytic degradation and detoxification of *o*-toluidine: Degradation mechanism and Salmonella mutagenicity assessment of mixed gaseous intermediates

► Two intermediates of toluene and phenol were found in the gas phase. ► Six trace amounts degradation intermediates were found on the surface of TiO<sub>2</sub>. ► *O*-Toluidine presented weak mutagenic activity against the TA100 strain with S9. ► Mutagenic toxicity of gaseous intermediates increased first and then decrease soon. ► Gaseous *o*-toluidine was successfully detoxified using photocatalytic technology.

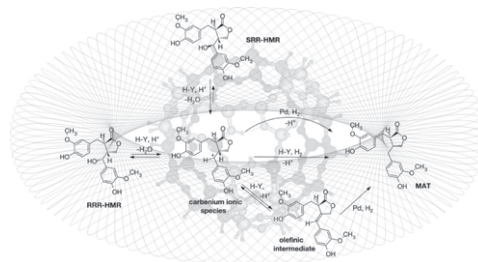


**Giampaolo Barone, Giovanni Li Manni, Antonio Prestianni, Dario Duca, Heidi Bernas, Dmitry Yu. Murzin**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 136

Hydrogenolysis of hydroxymatairesinol on Y derived catalysts: A computational study

► Hydrogenolysis of 7-hydroxymatairesinol to matairesinol occurs on Pd bifunctional catalysts. ► 7-hydroxymatairesinol naturally exists as a mixture of two diastereoisomers, RRR and SRR. ► In the hydrogenolysis, the SRR epimer is significantly more reactive than the RRR one. ► Many reaction paths may coexist, involving or not the catalytic Pd component. ► Palladium has a minor role in driving both the reaction rate and selectivity.

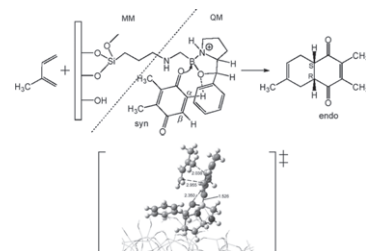


**Nasr Y.M. Omar, Noorsaadah A. Rahman, Sharifuddin Md Zain**

*Journal of Molecular Catalysis A: Chemical* 333 (2010) 145

An ONIOM study on the enantioselective Diels–Alder reaction catalyzed by SiO<sub>2</sub> – Immobilized chiral oxazaborolidinium cation

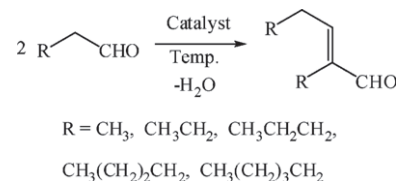
► SiO<sub>2</sub> surface is obtained by melt-quench method and resembles silica calcined at 673 K. ► Diels–Alder reaction on SiO<sub>2</sub> surface shows concerted highly asynchronous mechanism. ► The mechanism and enantioselectivity are comparable to homogeneous catalyst.



**Tharun Jose, N. Sudheesh, Ram S. Shukla***Journal of Molecular Catalysis A: Chemical* 333 (2010) 158

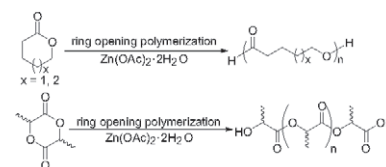
Amino functionalized chitosan as a catalyst for selective solvent-free self-condensation of linear aldehydes

► Aminopropyltrimethoxysilane functionalized chitosan. ► Efficient solid base catalyst. ► Selective solvent-free aldol condensation of linear aldehydes to  $\alpha,\beta$ -unsaturated aldehydes. ► Recyclability with no loss in activity up to six cycles.

**Ravikumar R. Gowda, Debashis Chakraborty***Journal of Molecular Catalysis A: Chemical* 333 (2010) 167

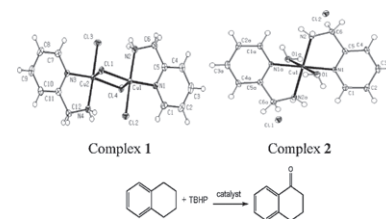
Zinc acetate as a catalyst for the bulk ring opening polymerization of cyclic esters and lactide

►  $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$  is found to be an effective bulk polymerization catalyst for the polymerization of cyclic esters and lactide. ► The major initiation pathway in the polymerization is found to proceed via the activated monomer mechanism. ► Polymers with different end groups can be synthesized. ► The overall system is green and eco friendly.

**Chunling Wang, Yuecheng Zhang, Baoguo Yuan, Jiquan Zhao***Journal of Molecular Catalysis A: Chemical* 333 (2010) 173

Synthesis, single crystal structures and efficient catalysis for tetralin oxidation of two novel complexes of Cu(II) with 2-aminomethyl pyridine

► Two novel Cu(II) complexes were synthesized and characterized thoroughly. ► Complex 1 showed high activity and selectivity in the tetralin oxidation by TBHP. ► Their catalysis in tetralin oxidation are related to the structure of the complexes.

**Gianni Cavinato, Sarah Facchetti, Luigi Toniolo***Journal of Molecular Catalysis A: Chemical* 333 (2010) 180

Ethene hydromethoxycarbonylation catalyzed by *cis*-[Pd(SO<sub>4</sub>)(PPh<sub>3</sub>)<sub>2</sub>]/H<sub>2</sub>SO<sub>4</sub>/PPh<sub>3</sub>

► [Pd(SO<sub>4</sub>)(PPh<sub>3</sub>)<sub>2</sub>]/H<sub>2</sub>SO<sub>4</sub>/PPh<sub>3</sub> catalyzes the hydromethoxycarbonylation of ethene. ► TOF = 2168 h<sup>-1</sup>, Pd/H<sub>2</sub>SO<sub>4</sub>/P = 1/107/18 (mol/mol), 6 bar (CO/E = 1/1). ► [Pd(SO<sub>4</sub>)(PPh<sub>3</sub>)<sub>2</sub>] in CD<sub>2</sub>Cl<sub>2</sub>/MeOH reacts with CO giving a Pd-CO complex. ► This species is unstable in the presence of H<sub>2</sub>O and H<sub>2</sub>SO<sub>4</sub> giving a Pd-H complex. ► The hydride complex yields catalysis in the presence of CO and ethene.

