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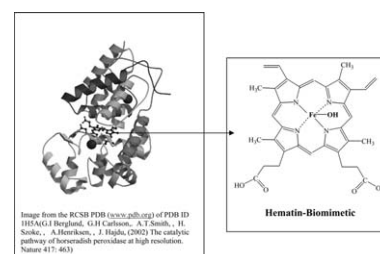
Articles

I. Magario, F.S. García Einschlag, E.H. Rueda, J. Zygodlo, M.L. Ferreira

Journal of Molecular Catalysis A: Chemical 352 (2012) 1

Mechanisms of radical generation in the removal of phenol derivatives and pigments using different Fe-based catalytic systems

► HRP, biomimetics and Fenton mechanism comparison of elimination of phenol and derivatives. ► Different results in phenolic compounds degradation with HRP depending on hydrogen peroxide concentration. ► Biomimetics lower activity but higher stability and minor cost than enzymes. ► Mechanisms between degradation to mineralization or oligo to polymerization depending on the system and experimental conditions.

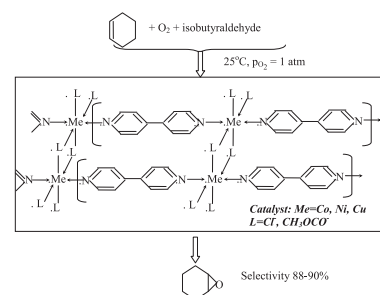


Emilian Angelescu, Octavian D. Pavel, Rodica Ionescu, Ruxandra Birjega, Mihaela Badea, Rodica Zăvoianu

Journal of Molecular Catalysis A: Chemical 352 (2012) 21

Transition metal coordination polymers $\text{MeX}_2(4,4'\text{-bipyridine})$ ($\text{Me} = \text{Co}, \text{Ni}, \text{Cu}$; $\text{X} = \text{Cl}^-, \text{CH}_3\text{OCO}^-, \text{acetylacetonate}$) selective catalysts for cyclohexene epoxidation with molecular oxygen and isobutyraldehyde

► $2_{\infty}[\text{Me}(\text{II})\text{Cl}_2(4,4'\text{-bipyridine})]$ show selectivity for cyclohexene epoxidation above 88% ► $2_{\infty}[\text{Co}(\text{II})\text{Cl}_2(4,4'\text{-bipyridine})]$ has better activity than analogous Ni or Cu complexes ► The presence of CH_3OCO^- instead of Cl^- in Co-complex increases the catalytic activity ► Replacement of Cl^- by acetylacetonate decreases the catalytic activity of Co-complex.

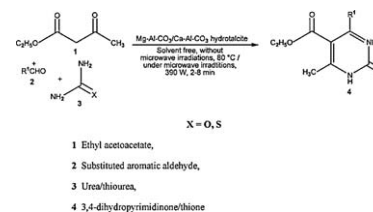


Jaggi Lal, Monika Sharma, Savita Gupta, Priyanka Parashar, Pramod Sahu, D.D. Agarwal

Journal of Molecular Catalysis A: Chemical 352 (2012) 31

Hydrotalcite: A novel and reusable solid catalyst for one-pot synthesis of 3,4-dihydropyrimidinones and mechanistic study under solvent free conditions

► This catalytic reaction takes place under solvent free conditions thus eliminating organic solvent, it gains an environment friendly condition. ► Yield of the desired product is excellent in the present synthesis. ► Hydrotalcite is a reusable heterogeneous catalyst there is no significant loss of catalytic activity when tested up to five catalytic cycles. ► Hydrotalcite catalyst containing Mg, Al and Ca are environment friendly metals.

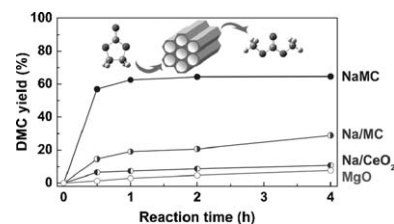


Tian-Tian Li, Lin-Bing Sun, Lu Gong, Xiao-Yan Liu, Xiao-Qin Liu

Journal of Molecular Catalysis A: Chemical 352 (2012) 38

In situ generation of superbasic sites on mesoporous ceria and their application in transesterification

► Solid superbasic materials were fabricated based on mesoporous ceria. ► In situ generation of superbasic sites in hard-templating synthetic system. ► Flexible utilization of basic solutions to remove template and function as guests. ► Excellent basic catalytic performance in dimethyl carbonate synthesis.

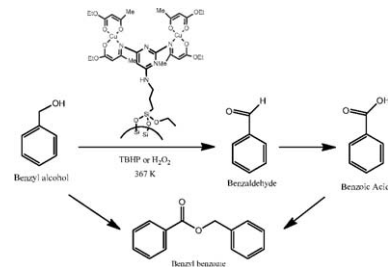


Yolanda Pérez, Ruth Ballesteros, Mariano Fajardo, Isabel Sierra, Isabel del Hierro

Journal of Molecular Catalysis A: Chemical 352 (2012) 45

Copper-containing catalysts for solvent-free selective oxidation of benzyl alcohol

► Copper metallic precursors have been immobilized onto previously organofunctionalized MCM-41 materials. ► The functionalized materials have been prepared by using both post-synthesis and co-condensation methods. ► Copper-containing catalysts have been tested in the benzyl alcohol oxidation under solventless conditions.

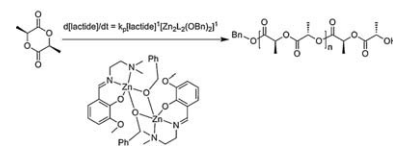


Lihui Yao, Lei Wang, Jinfeng Zhang, Ning Tang, Jincui Wu

Journal of Molecular Catalysis A: Chemical 352 (2012) 57

Ring opening polymerization of L-lactide by an electron-rich Schiff base zinc complex: An activity and kinetic study

► This zinc complex efficiently initiated the controlled polymerization of L-lactide. ► The introduction of methoxy at ortho-phenoxy leads to a decrease polymerization rate. ► The overall rate expression is $d[\text{lactide}]/dt = k_p[\text{lactide}]^2[\text{Zn}_2\text{L}_2(\text{OBn})_2]^1$.

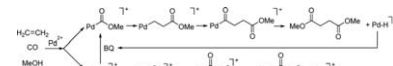


Gianni Cavinato, Sarah Facchetti, Luigi Toniolo

Journal of Molecular Catalysis A: Chemical 352 (2012) 63

Oxidative carbonylation of ethene catalyzed by Pd(II)-PPh₃ complexes in MeOH using benzoquinone as stoichiometric oxidant

► Pd²⁺/benzoquinone in MeOH catalyze the ethene carbonylation to dimethyl succinate. ► Other products are dimethyl-carbonate, -oxalate and methyl propanoate. ► In the absence of benzoquinone catalysis yields methyl propanoate. ► Benzoquinone switches catalysis from the Pd-H mechanism to the Pd-COOMe one.

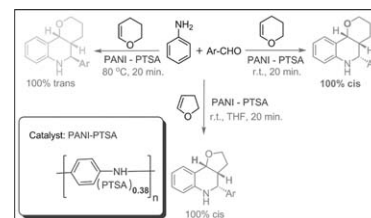


Srinivasan Palaniappan, Boddula Rajender, Male Umashankar

Journal of Molecular Catalysis A: Chemical 352 (2012) 70

Controllable stereoselective synthesis of *cis* or *trans* pyrano and furano tetrahydroquinolines: Polyaniline-*p*-toluenesulfonate salt catalyzed one-pot aza-Diels-Alder reactions

► PANI-PTSA serves as reusable catalyst to pre-pare *cis* or *trans* tetrahydroquinolines. ► *cis* or *trans* products were obtained by controlling the reaction temperature. ► Tetrahydroquinolines were obtained in a very short time.

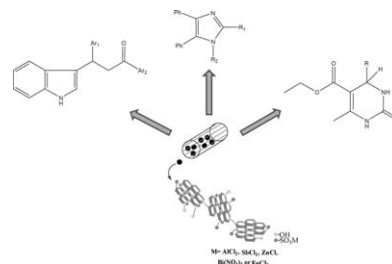


Princy Gupta, Satya Paul

Journal of Molecular Catalysis A: Chemical 352 (2012) 75

Sulfonated carbon/silica composite functionalized Lewis acids for one-pot synthesis of 1,2,4,5-tetrasubstituted imidazoles, 3,4-dihydropyrimidin-2(1H)-ones and for Michael addition of indole to α,β -unsaturated ketones

► Sulfonated carbon/silica functionalized Lewis acids were prepared from starch. ► Different Lewis acids were tested with a view to select the most active solid acid. ► Lewis acid catalysts were characterized by FTIR, XRD and AAS analysis. ► Most active catalyst CSC-Star-SO₃-AlCl₂ was also characterized by TGA, SEM and TEM. ► CSC-Star-SO₃-AlCl₂ was found to be recyclable under the reaction conditions.

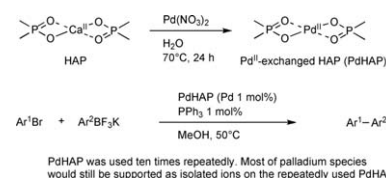


Yoshiro Masuyama, Yutaka Sugioka, Shiori Chonan, Noriyuki Suzuki, Masahiro Fujita, Kenji Hara, Atsushi Fukuoka

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Palladium(II)-exchanged hydroxyapatite-catalyzed Suzuki-Miyaura-type cross-coupling reactions with potassium aryltrifluoroborates

► Pd(II)-exchanged hydroxyapatite catalyzed Suzuki-Miyaura cross-coupling reaction. ► The coupling reaction was carried out in methanol under air. ► The heterogeneous Pd catalyst was used ten times repeatedly. ► Most of Pd species would still be supported as isolated ions in repetitive uses.

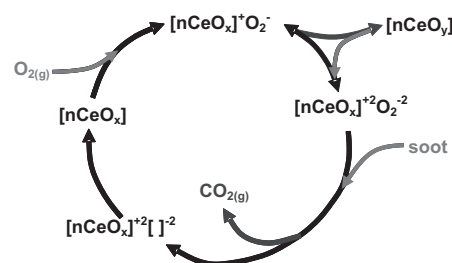


Martín S. Gross, María A. Ulla, Carlos A. Querini

Journal of Molecular Catalysis A: Chemical 352 (2012) 86

Diesel particulate matter combustion with CeO₂ as catalyst. Part I: System characterization and reaction mechanism

► Soot oxidation on ceria occurs by a mechanism involving superoxides and peroxides species. ► Calcination temperature and operation temperature affect the concentration of these species. ► The mechanism explains the transient kinetic behavior.

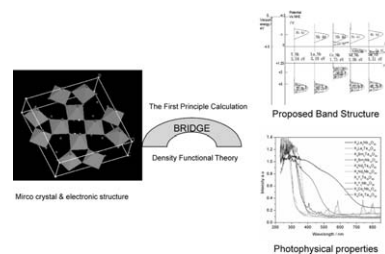


**Mengkui Tian, Wenfeng Shangguan,
Wenliang Tao**

Journal of Molecular Catalysis A: Chemical 352 (2012) 95

The photocatalytical activities for water decomposition of $K_4R_2M_{10}O_{30}$ (R = Y, La, Ce, Nd, Sm; M = Ta, Nb) and their photophysical properties based on the first principle calculation

► Photocatalysts $K_4R_2M_{10}O_{30}$ (R = Y, La, Ce, Nd, Sm; M = Ta, Nb) were presented. ► These photo-catalysts showed water decomposition activities under $\lambda > 300$ nm. ► Only R = Ce showed photo-catalytical activities under $\lambda > 420$ nm. ► Their electronic structures were studied based on the first principle calculation. ► The band structures were proposed and showed good agreement with activities.

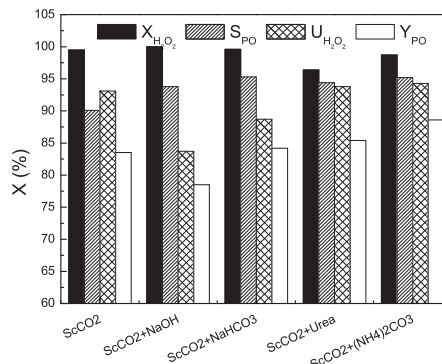


**Yu Chen, Yulong Wu, Yaori Zhang, Liang Long,
Ling Tao, Mingde Yang, Na Tang**

Journal of Molecular Catalysis A: Chemical 352 (2012) 102

Epoxidation of propylene to propylene oxide catalyzed by large-grain TS-1 in supercritical CO_2

► Large grain size TS-1 was introduced to propylene epoxidation. ► It is concluded that the large grain size TS-1 has important roles on propylene epoxidation in $scCO_2$. ► Environmental-friendly $scCO_2$ substituted for MeOH as reaction medium and increased the catalytic activity of large grain size TS-1. ► $(NH_4)_2CO_3$ as additive improved the selectivity and yield of propylene oxide in $scCO_2$. ► The maximum conversion of H_2O_2 , selectivity of PO, utilization of H_2O_2 , and yield of PO were 98.7%, 95.2%, 94.3% and 88.6% respectively in $scCO_2$ with alkaline component as additives.

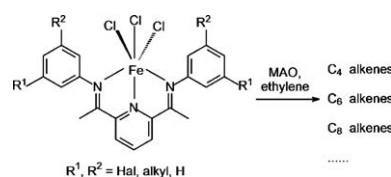


**Christian Görl, Nadine Beck, Katharina Kleiber,
Helmut G. Alt**

Journal of Molecular Catalysis A: Chemical 352 (2012) 110

Iron(III) complexes with *meta*-substituted bis(arylimino)pyridine ligands: Catalyst precursors for the selective oligomerization of ethylene

► Synthesis of highly selective bis(arylimino)pyridine iron(III) catalysts for the oligomerization of ethylene to short chain α -olefins. ► Detailed description of the influence of the substitution patterns of the ligand back-bones on the catalytic behavior. ► Surprising production of internal and branched olefins: isomerization, copolymerization and unusual reaction pathways.



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

Journal of Molecular Catalysis A: Chemical 352 (2012) 128

Palladium nanoparticle supported on cobalt ferrite: An efficient magnetically separable catalyst for ligand free Suzuki coupling

► A Pd-CoFe₂O₄ magnetic nanocomposite with-out any capping agent. ► Pd nanoparticles are supported *in situ* during CoFe₂O₄ nanoparticle synthesis. ► Nanoparticles are stable in polar solvents such as water and ethanol. ► Pd-CoFe₂O₄ catalyzes Suzuki reaction in ethanol under ligand free condition ► Magnetic nanocomposite could be recovered using an external magnet and reused.

