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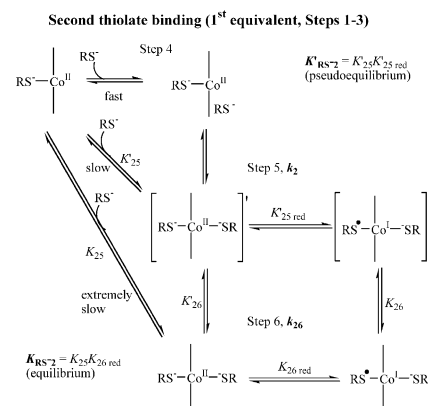
Articles

Eduard M. Tyapochkin, Evguenii I. Kozliak

Journal of Molecular Catalysis A: Chemical 242 (2005) 1

Kinetic and binding studies of the thiolate–cobalt tetrasulfophthalocyanine anaerobic reaction as a subset of the Merox process

Thiolate binding to cobalt tetrasulfophthalocyanine (CoTSPc) is a multi-step process with the intermediate formation of outer-sphere complexes. Binding of the second thiolate occurs when CoTSPc is oligomeric (in aqueous media) and is accompanied by pronounced cobalt(II) reduction (rate-limiting step). This anaerobic process, including the 2:1 thiolate–CoTSPc stoichiometry, is a subset of the aerobic Merox process (CoTSPc-catalyzed thiolate autoxidation).

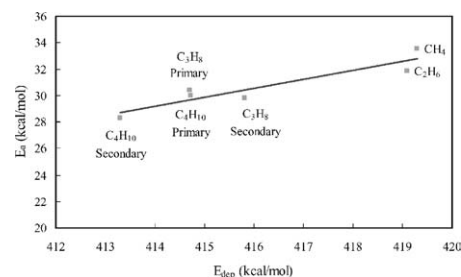


Xiaobo Zheng, Paul Blowers

Journal of Molecular Catalysis A: Chemical 242 (2005) 18

A computational study of alkane hydrogen-exchange reactions on zeolites

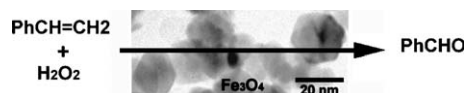
In this work, zeolite-catalyzed light alkane hydrogen-exchange reactions, including methane, ethane, propane, and butane, are investigated using ab initio quantum chemical methods. Applying the cluster approach method, the activation energies for each reaction are calculated and compared with available experimental and computational data. A linear relationship between the activation energy, E_a , and the deprotonation energy, E_{dep} , is proposed and shown below.



Debanjan Guin, Babita Baruwati, Sunkara V. Manorama

Journal of Molecular Catalysis A: Chemical 242 (2005) 26

A simple chemical synthesis of nanocrystalline AFe_2O_4 ($A = Fe, Ni, Zn$): An efficient catalyst for selective oxidation of styrene

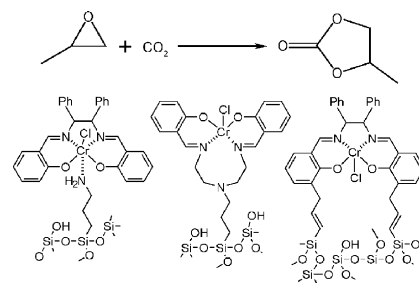


**Michael Ramin, Fabian Jutz,
Jan-Dierk Grunwaldt, Alfons Baiker**

Journal of Molecular Catalysis A: Chemical 242 (2005) 32

Solventless synthesis of propylene carbonate catalysed by chromium–salen complexes: Bridging homogeneous and heterogeneous catalysis

Various chromium complexes were synthesised and tested concerning their catalytic performance in the synthesis of propylene carbonate from carbon dioxide and propylene oxide. The most active complexes were immobilised on a silica support and tested in the same reaction. Different immobilisation methods were applied (figure). The coordinatively-bound complexes showed low stability and a very strong deactivation during reuse, whereas the corresponding covalently-bound complexes hardly showed any chromium leaching during catalyst recycling experiments.

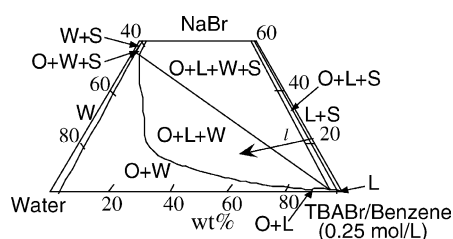


**Noritaka Ohtani, Tsuyoshi Yamashita,
Tomoaki Ohta, Yasuhiro Hosoda**

Journal of Molecular Catalysis A: Chemical 242 (2005) 40

Phase-behavior and solid–liquid phase-transfer catalytic activity of tetrabutylammonium bromide

The addition of water to TBABr/benzene/NaBr systems induced the separation of TBABr-rich liquid phase (L phase) prior to the appearance of an aqueous phase (W phase). The L phase was assumed to be similar to a bicontinuous microemulsion based on the phase composition. TBABr catalyzed the “solid–liquid” phase-transfer reaction of decyl methanesulfonate with NaBr only when the L phase was fully hydrated.

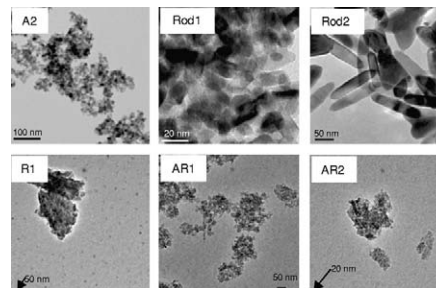


**Rajeev K. Wahi, William W. Yu, Yunping Liu,
Michelle L. Mejia, Joshua C. Falkner,
Whitney Nolte, Vicki L. Colvin**

Journal of Molecular Catalysis A: Chemical 242 (2005) 48

Photodegradation of Congo Red catalyzed by nano-sized TiO₂

Anatase TiO₂ is a superior photocatalyst to rutile TiO₂ due to the inherent difference in the two crystal structures. Anatase TiO₂ nanorods with predominantly (1 0 1) surface exhibited low activity because the non-dissociative adsorption of H₂O to this surface retarded the generation of OH[•] radicals required for facile photocatalytic oxidation. TiO₂ nanocrystal shapes significantly affected their photocatalytic activities.

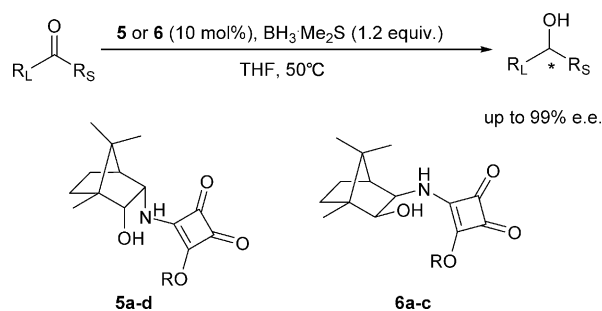


**Hai-Hua Zou, Jian Hu, Ji Zhang,
Jing-Song You, Dan Ma, Ding Lü, Ru-Gang Xie**

Journal of Molecular Catalysis A: Chemical 242 (2005) 57

Asymmetric reduction of prochiral ketones with borane using chiral squaric amino alcohols derived from camphor as catalysts

A series of new chiral squaric amino alcohols derived from (*R*)-(+)-camphor and squaric acid were synthesized, and applied to the enantioselective reduction of prochiral ketones with borane to give secondary alcohols with excellent enantiomeric excesses (up to 99%).

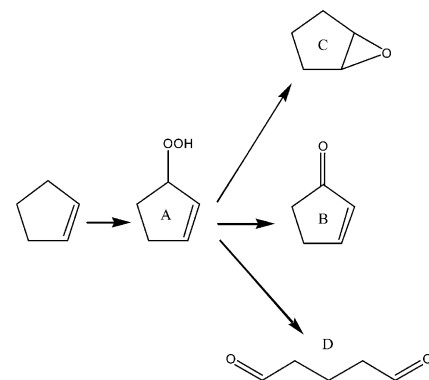


**Petr Kluson, Hana Luskova, Libor Cervený,
Jana Klisakova, Tomas Cajthaml**

Journal of Molecular Catalysis A: Chemical 242
(2005) 62

Partial photocatalytic oxidation of cyclopentene
over titanium(IV) oxide

In analogy with cyclohexane, a group of oxidation products appeared mainly including cyclopent-2-en-1-one (in much lower quantities also cyclopent-2-en-1-ol). The epoxide fraction involved mostly 6-oxabicyclo[3.1.0]hexane, appearance of other products of this type was marginal.

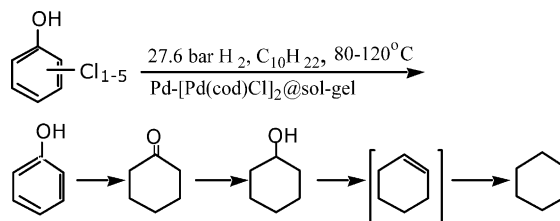


**Tatiana Tehila Bovkun, Yoel Sasson,
Jochanan Blum**

Journal of Molecular Catalysis A: Chemical 242
(2005) 68

Conversion of chlorophenols into cyclohexane by a
recyclable Pd-Rh catalyst

In the presence of a silica sol-gel entrapped catalyst composed of metallic palladium and $[\text{Rh}(\text{cod})(\mu\text{-Cl})_2]$ under 27.6 bar H_2 at 120°C mono-, di-, tri- and tetrachlorophenols undergo exhaustive hydrogenation to give cyclohexane in $>95\%$ yield. The main isolated intermediates in this process, which can be isolated at lower temperatures are phenol, cyclohexanone and cyclohexanol. The combined entrapped catalyst is leach-proof and recyclable without loss in catalytic activity in three to six runs.

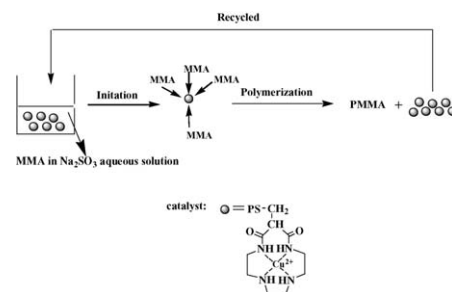


**Jianmei Lu, Qingfeng Xu, Yuanqing Xu,
Najun Li, Yesu Guo**

Journal of Molecular Catalysis A: Chemical 242
(2005) 74

Polystyrene copper(II) complex containing aza-
crown ether functional groups as catalyst for room-
temperature polymerization of MMA

A surface-modified cross-linked polystyrene metal complex (PS-DCTACE-Cu(II)) is applied as catalyst of methyl methacrylate (MMA) heterogeneous polymerization at ambient temperature in Na_2SO_3 aqueous solution. The catalyst has excellent mechanical property and is easy to be separate from reaction system and recycled. The mechanism of polymerization, a process of 'chloridion leaving-hydrogen transfer', was also studied in this paper.

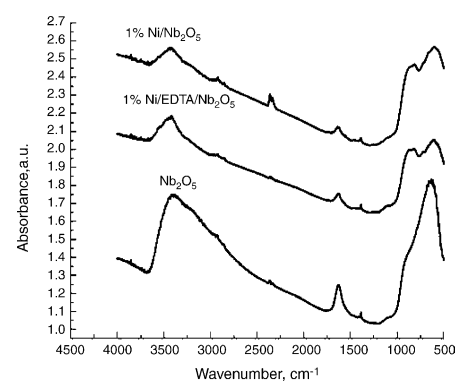


**A. Jasik, R. Wojcieszak, S. Monteverdi,
M. Ziolk, M.M. Bettahar**

Journal of Molecular Catalysis A: Chemical 242
(2005) 81

Study of nickel catalysts supported on Al_2O_3 , SiO_2
or Nb_2O_5 oxides

Nickel classical catalysts supported on Al_2O_3 , SiO_2
and Nb_2O_5 were prepared using simple or EDTA-
double impregnation methods. Non-classical cata-
lysts were obtained by pretreatment of the nickel
precursors in aqueous hydrazine. The surface and
catalytic properties were found to be determined by
metal-support interactions which, in turn, were
influenced by the method of preparation or nature of
the support.

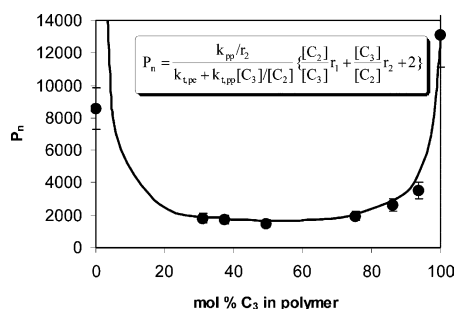


**Nic Friederichs, Bing Wang,
Peter H.M. Budzelaar, Betty B. Coussens**

Journal of Molecular Catalysis A: Chemical 242 (2005) 91

A combined experimental—molecular modeling approach for ethene–propene copolymerization with C_2 -symmetric metallocenes

Trends in molecular weight for ethene/propene copolymerization using C_2 -symmetric zirconocenes can be well described by combining experimental r_2 parameters with calculated barriers for propene insertion and chain transfer to both monomers.



**Nan Jiang, Shuping Yuan, Jianguo Wang,
Zhangfeng Qin, Haijun Jiao**

Journal of Molecular Catalysis A: Chemical 242 (2005) 105

Amines adsorption on Li- and Na-exchanged MOR: An ONIOM2 Study

The adsorption of amines (NH_3 , NH_2Me , $NHMe_2$ and NMe_3) on Li- and Na-exchanged MOR was investigated by the ONIOM2 method. The coordination of amine nitrogen to the alkali cation in zeolite dominates the overall interaction, and the adsorption complexes are further stabilized by weak hydrogen bonding between amine and zeolite framework oxygen atoms. The adsorption energy of amines on Li- and Na-MOR only amounts to about 63–72 and 71–87% of the binding energy of the naked Li^+ and Na^+ with amines, respectively.



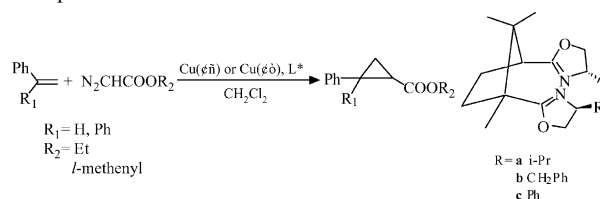
**Qitao Tan, Jiwu Wen, Daliang Li, Hongyan Li,
Tianpa You**

Journal of Molecular Catalysis A: Chemical 242 (2005) 113

Novel bis(oxazoline) ligands derived from camphoric acid for Cu-catalyzed asymmetric cyclopropanation

Novel bis(oxazoline) ligands were prepared and applied to Cu-catalyzed asymmetric cyclopropanation of styrene and 1,1-diphenylethylene with diazoacetate.

Novel bis(oxazoline) ligands with additional chiral centers in the linker between the oxazoline groups were conveniently synthesized and applied to Cu-catalyzed asymmetric cyclopropanation of olefin with diazoacetate. Enantiomeric excess up to 81% was obtained for 1,1-diphenylethylene; however, the enantioselectivity for styrene was poor. The chiral centers in the oxazoline group controlled the configuration of the products, while no significant matching or mismatching problem between the chiral centers of the main oxazoline groups and the camphor backbone was observed.

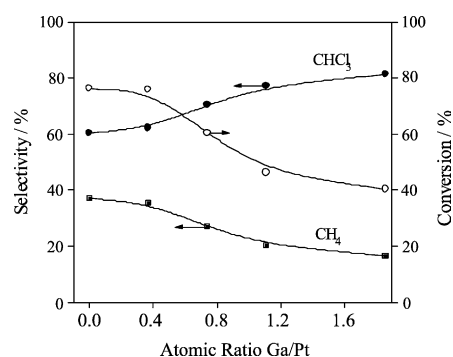


Yu Cai Cao, Xuan Zhen Jiang

Journal of Molecular Catalysis A: Chemical 242 (2005) 119

Supported platinum–gallium catalysts for selective hydrodechlorination of CCl_4

The selective hydrodechlorination of tetrachloromethane (CCl_4) was performed over supported platinum–gallium catalysts to improve $CHCl_3$ selectivity and catalytic stability. The Ga addition will significantly increase the dispersion of Pt and create more Pt sites on the catalyst surface. The influence of Ga on the selectivity and conversion can be ascribed to its modification to the electronic properties of Pt.

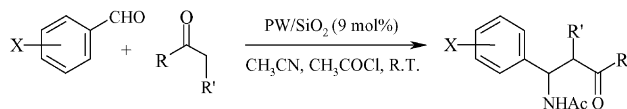


**Ezzat Rafiee, Fomaida Shahbazi,
Mohammad Joshaghani, Fariba Tork**

Journal of Molecular Catalysis A: Chemical 242 (2005) 129

The silica supported $H_3PW_{12}O_{40}$ (a heteropoly acid) as an efficient and reusable catalyst for a one-pot synthesis of β -acetamido ketones by Dakin–West reaction

Heteropoly acid $H_3PW_{12}O_{40}$ (PW) supported on silica (PW/SiO₂) as an efficient, reusable solid acid catalyst have been studied in the one-pot, four-component coupling process for the synthesis of β -acetamido ketones.

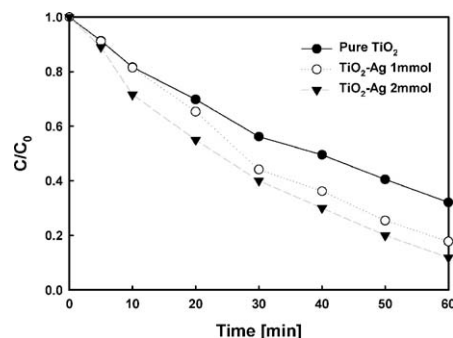


Man Sig Lee, Seong-Soo Hong, Madjid Mohseni

Journal of Molecular Catalysis A: Chemical 242 (2005) 135

Synthesis of photocatalytic nanosized TiO₂-Ag particles with sol-gel method using reduction agent

TiO₂-Ag nanoparticles were prepared with the sol-gel method using a reduction agent. The major phase of all the prepared TiO₂-Ag nanoparticles was anatase structure regardless of the AgNO₃ content. TiO₂-Ag nanoparticles possessed a spherical morphology with a narrow size distribution. Also, the presence of Ag improved the photocatalytic activity of TiO₂-Ag and the photodegradation of model contaminant *p*-nitrophenol.

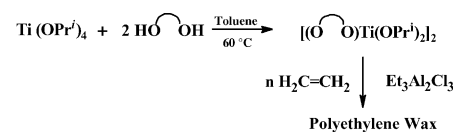


**P.S. Umare, R. Antony, K. Gopalakrishnan,
G.L. Tembe, B. Trivedi**

Journal of Molecular Catalysis A: Chemical 242 (2005) 141

Synthesis of low molecular weight polyethylene waxes by a titanium BINOLate-ethylaluminum sesquichloride catalyst system

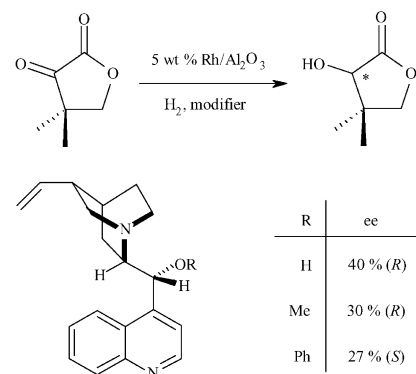
Homogeneous titanium (IV) complexes of chiral ligand Binol which can be synthesized conveniently from readily available starting materials in combination with alkyl aluminum sesquichloride (Et₃Al₂Cl₃) as co-catalyst selectively polymerize ethylene at elevated temperatures to highly crystalline low molecular weight polyethylene waxes with narrow polydispersity. These specialty waxes have potential applications in surface coating and ink formulations.



Mihaela Maris, Tamas Mallat, Alfons Baiker

Journal of Molecular Catalysis A: Chemical 242 (2005) 151

Rhodium-catalyzed enantioselective hydrogenation of ketopantolactone

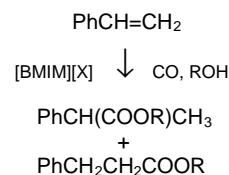


Gábor Rangits, László Kollár

Journal of Molecular Catalysis A: Chemical 242 (2005) 156

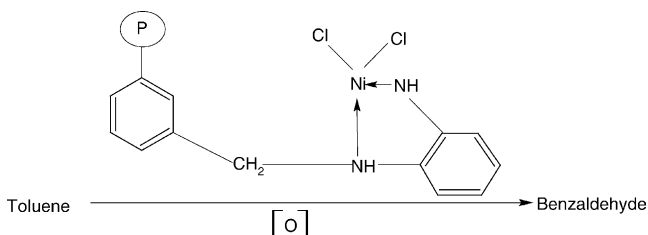
Palladium-catalysed hydroalkoxycarbonylation of styrene in [BMIM][BF₄] and [BMIM][PF₆] ionic liquids

The hydroalkoxycarbonylation of styrene was carried out by using various alcohols (ethanol, *n*- and *i*-propyl alcohol, benzyl alcohol, *n*-octyl alcohol) in imidazolium-based ionic liquids.

**Kamlesh Gauli, R.N. Ram, Hemant P. Soni**

Journal of Molecular Catalysis A: Chemical 242 (2005) 161

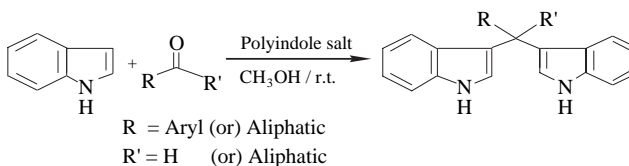
Oxidation of toluene using polymer anchored Ni(II) complex as catalyst

**Srinivasan Palaniappan, Amalraj John**

Journal of Molecular Catalysis A: Chemical 242 (2005) 168

Facile synthesis of bis(indolyl)methanes using polyindole salt as reusable catalyst

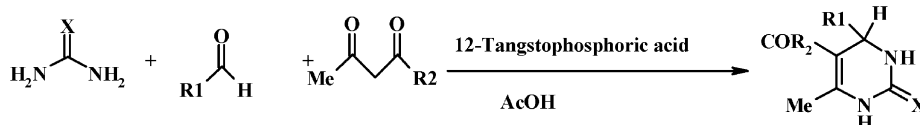
Polyindole salt was used as an efficient catalyst for the synthesis of bis(indolyl)methanes for the first time and afford excellent yield in room temperature. Furthermore, after completion of reaction the catalyst could be easily recovered and can be reused.

**Majid M. Heravi, Fatemeh Derikvand, Fatemeh F. Bamoharram**

Journal of Molecular Catalysis A: Chemical 242 (2005) 173

A catalytic method for synthesis of Biginelli-type 3,4-dihydropyrimidin-2(1H)-one using 12-tungstophosphoric acid

A simple, efficient and cost-effective method for the synthesis of 3,4-dihydropyrimidin-2(1H)-one by a one-pot three-component cyclocondensation reaction of a 1,3-dicarbonyl compound, an aldehyde and urea or thiourea using 12-tungstophosphoric acid as a recyclable catalyst is reported.

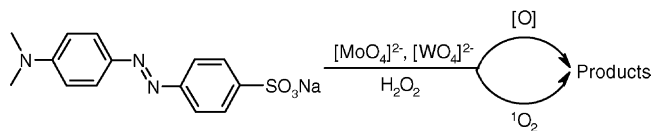


**David M. Gould, Michael Spiro,
William P. Griffith**

Journal of Molecular Catalysis A: Chemical 242 (2005) 176

Mechanism of bleaching by peroxides. Part 7. The pH dependence of the oxometalate catalysed bleaching of methyl orange

Kinetics and mechanisms of the bleaching of methyl orange by H_2O_2 catalysed by MoO_4^{2-} and WO_4^{2-} have been studied from pH 8.95 to 11.0 in a variety of buffers. Contributory rate constants for both the peroxometalate catalyst and the singlet oxygen pathways were determined from experiments both without and with the singlet oxygen trap 2,5-dimethylfuran. The variation with pH of the singlet oxygen rate constants correlated well with $^1\text{O}_2$ generation rates in the literature.

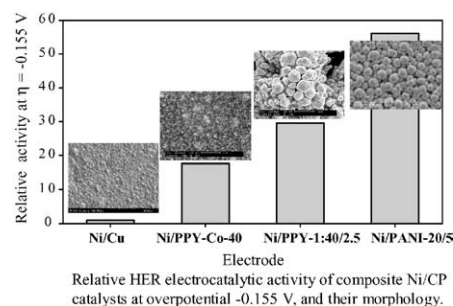


Elisa Navarro-Flores, Sasha Omanovic

Journal of Molecular Catalysis A: Chemical 242 (2005) 182

Hydrogen evolution on nickel incorporated in three-dimensional conducting polymer layers

Conducting polymers (CP), polypyrrole (PPY), and polyaniline (PANI) are used as three-dimensional patterning templates (matrices) for electrodeposition of nickel on an inert glassy carbon surface. It is shown that Ni/CP layers offer a significantly higher overall electrocatalytic activity in the hydrogen evolution reaction (HER) than Ni electrodeposited on a flat two-dimensional substrate. This is a result of favorable Ni/CP morphology which yields an increase in the active surface area of the catalyst.

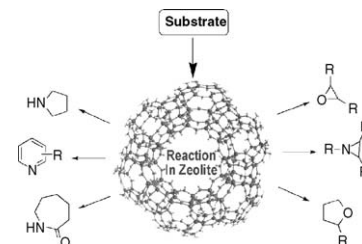


Nuno R. Candeias, Carlos A.M. Afonso

Journal of Molecular Catalysis A: Chemical 242 (2005) 195

Preparation of non-fused heterocycles in zeolites and mesoporous materials

The use of zeolites and mesoporous materials in synthesis and industrial applications are extremely important due to their acidity properties and their reuse facility. In this review, is presented the use of zeolites and mesoporous materials in the preparation of non-fused heterocycles compounds, with particular emphasis in epoxidations, aziridinations and the Beckmann's rearrangement.

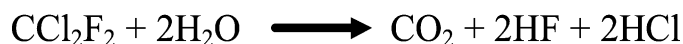


**Jie Zhao, Bozhi Tian, Yinghong Yue,
Weiming Hua, Dongyuan Zhao, Zi Gao**

Journal of Molecular Catalysis A: Chemical 242 (2005) 218

New catalysts for dichlorodifluoromethane hydrolysis: Mesostructured titanium and aluminum phosphates

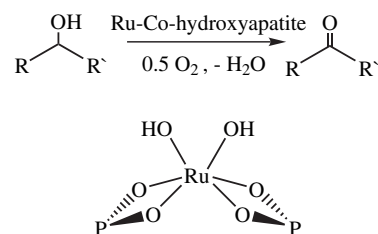
The catalytic hydrolysis of CCl_2F_2 over mesoporous metal phosphates is reported and compared with ordinary metal phosphates. The former catalysts are much more active than the latter ones. The activity of the catalysts is correlated with their surface acidity and hydroxyl groups.



Z. Opre, J.-D. Grunwaldt, T. Mallat, A. Baiker

Journal of Molecular Catalysis A: Chemical 242 (2005) 224

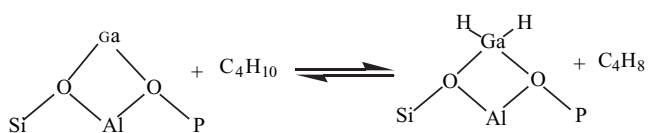
Selective oxidation of alcohols with oxygen on Ru–Co-hydroxyapatite: A mechanistic study



Anibal Sierraalta, Yajaira Guillen, Carmen M. López, Ramon Martinez, Fernando Ruetze, Francisco Machado, Marcos Rosa-Brussin, Humberto Soscún

Journal of Molecular Catalysis A: Chemical 242 (2005) 233

Theoretical study of the Ga/SAPO-11 catalyst. Extra-framework gallium species and *n*-butane transformation

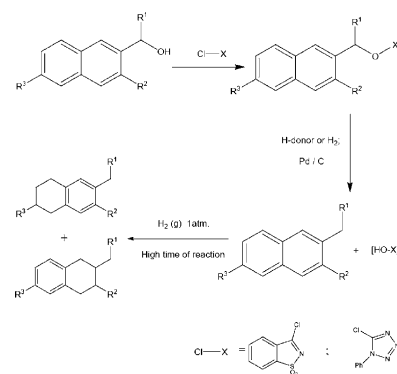


Luís M.T. Frija, M. Lurdes S. Cristiano, Emanuel M.O. Guimarães, Nelson C. Martins, Rui. M.S. Loureiro, Jamie F. Bickley

Journal of Molecular Catalysis A: Chemical 242 (2005) 241

Palladium-catalysed reduction of heteroaromatic naphthyl ethers: Structural effects on reactivity

Experimental conditions for palladium-catalysed hydrogenolysis of tetrazolyl and benzisothiazolyl naphthylmethylic ethers, with a hydrogen donor and with molecular hydrogen, were investigated. Analysis of the structure and reactivity indicates that these compounds are structurally similar to the corresponding benzyloxyderivatives around the ether bond but exhibit different reactivity. It can be concluded from this investigation that 5-chloro-1-phenyltetrazole acts as a better derivatizing agent for naphthyl methanols than 3-chloro-1,2-benzisothiazole-11-dioxide, this contrasting with what has been observed with phenols, allylic and benzylic alcohols.



Valiollah Mirkhani, Shahram Tangestaninejad, Majid Moghadam, Iraj Mohammadpoor-Baltork, Hadi Kargar

Journal of Molecular Catalysis A: Chemical 242 (2005) 251

Efficient oxidation of sulfides with sodium periodate catalyzed by manganese(III) Schiff base complexes

In the chemical system containing Mn(III)–salophen complex as catalyst, sulfides were converted efficiently to the corresponding sulfoxides and sulfones with sodium periodate. The ability of various Schiff base complexes in the oxidation of sulfides was also investigated.

