



Contents

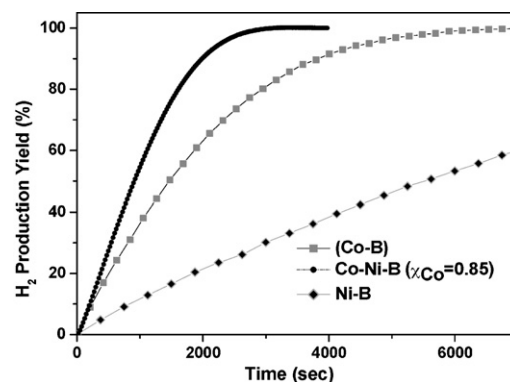
Articles

R. Fernandes, N. Patel, A. Miotello, M. Filippi

Journal of Molecular Catalysis A: Chemical 298 (2009) 1

Studies on catalytic behavior of Co–Ni–B in hydrogen production by hydrolysis of NaBH_4

Co–Ni–B with the $\text{Co}/(\text{Co} + \text{Ni})$ molar ratio (χ_{Co}) of 0.85 exhibited much superior activity than that of Co–B and Ni–B with highest H_2 generation rate obtained by the hydrolysis of NaBH_4 . The enhanced activity could be attributed to: large active surface area, amorphous short range structure and electron transfer by alloying large quantity of B to active Co and Ni sites on the surface of the catalyst.

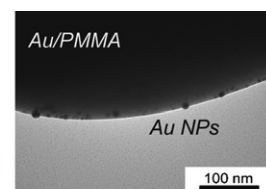
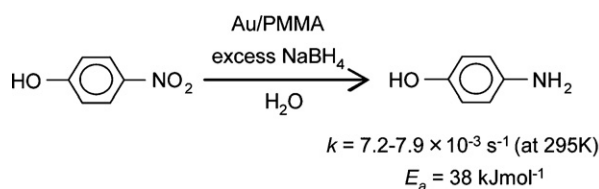


Kyoko Kuroda, Tamao Ishida, Masatake Haruta

Journal of Molecular Catalysis A: Chemical 298 (2009) 7

Reduction of 4-nitrophenol to 4-aminophenol over Au nanoparticles deposited on PMMA

Catalytic activity of Au nanoparticles deposited on PMMA was tested for the reduction of 4-nitrophenol to 4-aminophenol with an excess amount of NaBH_4 . Gold on PMMA was as active as the highest catalytic performance among polymer supported Au nanoparticles reported so far. The pseudo-first-order rate constant and the activation energy were $7.2\text{--}7.9 \times 10^{-3} \text{ s}^{-1}$ at 295 K and 38 kJ mol^{-1} , respectively.

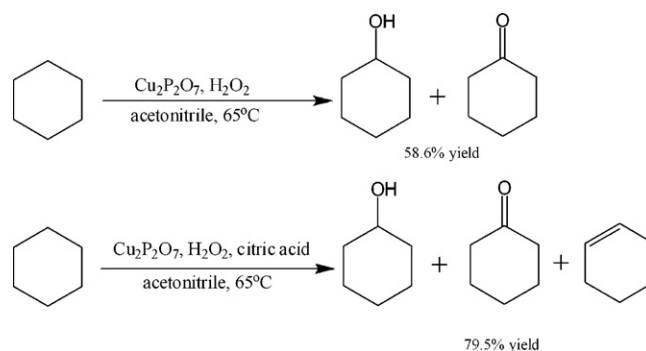


Ying Du, Yonglian Xiong, Jing Li, Xiangguang Yang

Journal of Molecular Catalysis A: Chemical 298 (2009) 12

Selective oxidation of cyclohexane with hydrogen peroxide in the presence of copper pyrophosphate

Liquid phase oxidation of cyclohexane was carried out over copper pyrophosphate catalyst using hydrogen peroxide as an oxidant in CH_3CN at the temperature between 25 and 80°C . It was found that appropriate surface hydrophobicity is the key factor for the excellent performance of the catalyst. Additionally, a significant improvement for the cyclohexane conversion in the presence of organic acid was observed.

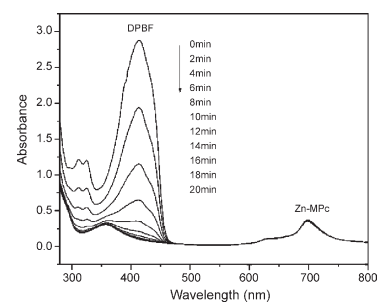


Xiaoyuan Shen, Wangyang Lu, Guihua Feng, Yuyuan Yao, Wenxing Chen

Journal of Molecular Catalysis A: Chemical 298 (2009) 17

Preparation and photoactivity of a novel water-soluble, polymerizable zinc phthalocyanine

Modification of zinc tetraaminophthalocyanine with maleic anhydride afforded a water-soluble, polymerizable zinc tetra(*N*-carbonylacrylic)aminophthalocyanine. It is an efficient photosensitizer in terms of the rate of DPBF degradation and the photostability. The kinetics equation of the initial degradation rate of DPBF is $R_d = 1.12 \times 10^{-5} [\text{DPBF}]^{0.51} [\text{Zn-MPc}]^{0.54} I^{1.35}$, which can provide a novel thought for the application of photosensitizers in PDT and the design of other efficient photosensitizers.

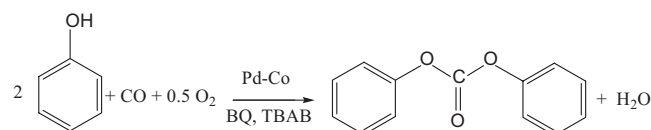


L. Ronchin, A. Vavasori, E. Amadio, G. Cavinato, L. Toniolo

Journal of Molecular Catalysis A: Chemical 298 (2009) 23

Oxidative carbonylation of phenols catalyzed by homogeneous and heterogeneous Pd precursors

Homogeneous and heterogeneous Pd-based catalysts (in the presence of $\text{Co}(\text{acac})_3/\text{ligand}/\text{BQ}/\text{TBAB}$ and molecular sieve 4A), have been compared in the oxidative carbonylation of phenols to diphenylcarbonate (DPC). In 4 h of reaction similar behavior in terms of yield and selectivity in DPC has been observed, on the contrary, in 20 h, only the systems $\text{Pd}(\text{OAc})_2/\text{Co}(\text{acac})_3/\text{dmphen}/\text{BQ}/\text{TBAB}$ and $\text{Pd}(\text{OAc})_2/\text{Co}(\text{acac})_3/\text{triind}/\text{BQ}/\text{TBAB}$ double the yield in DPC. The beneficial effect of the ligands and of TBAB might be due to their capacity of inhibiting the growing of Pd nanoparticles, thus easing their reoxidation to Pd(II) species. The initial rate of phenol or methyl substituted phenols in CH_2Cl_2 as a solvent is only slightly influenced, except in the case of bulkier 2,6-dimethyl phenol. The conversion vs. time profile evidences that fast catalyst deactivation occurs in any case.

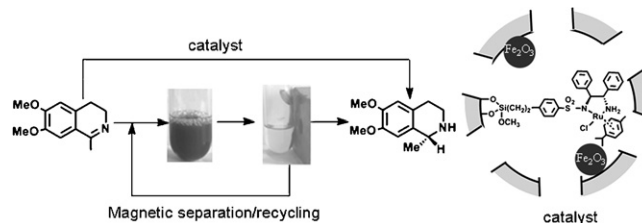


Jun Li, Yanmei Zhang, Difei Han, Qiang Gao, Can Li

Journal of Molecular Catalysis A: Chemical 298 (2009) 31

Asymmetric transfer hydrogenation using recoverable ruthenium catalyst immobilized into magnetic mesoporous silica

A ruthenium complex catalyst was firstly immobilized in the magnetic siliceous mesocellular foam material. This immobilized catalyst afforded high catalytic activities and good enantioselectivities in the asymmetric transfer hydrogenation of imine in $\text{HCOOH-Et}_3\text{N}$ system and aromatic ketones in aqueous HCOONa . Furthermore, this heterogeneous catalyst showed an excellent durability and can be reused conveniently by external magnet for at least nine times without noticeable loss of ee value.

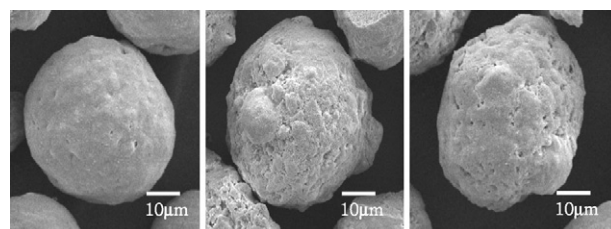


Eonah Kim, Eun Woo Shin, Ik-Keun Yoo, Jin Suk Chung

Journal of Molecular Catalysis A: Chemical 298 (2009) 36

Characteristics of heterogeneous titanium alkoxide catalysts for ring-opening polymerization of lactide to produce polylactide

$\text{TiCl}(\text{O-}i\text{-Pr})_3/\text{SiO}_2$ and $\text{Ti}(\text{O-}i\text{-Pr})_4/\text{SiO}_2$ were prepared by immobilizing titanium(IV) chloride triisopropoxide ($\text{TiCl}(\text{O-}i\text{-Pr})_3$) and titanium(IV) tetraisopropoxide ($\text{Ti}(\text{O-}i\text{-Pr})_4$), respectively, over-pretreated silica for ring-opening polymerization of lactide to produce polylactide. The PLA produced using silica-supported alkoxide catalysts had a higher molecular weight and T_m than those produced with the homogeneous catalyst.

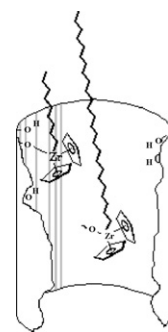


Fernando Silveira, Maria do Carmo Martins Alves, Fernanda C. Stedile, Sibe B. Pergher, Arnaud Rigacci, João Henrique Zimnoch dos Santos

Journal of Molecular Catalysis A: Chemical 298 (2009) 40

Effect of the silica texture on the structure of supported metallocene catalysts

The textural parameters of silicas, employed as supports for metallocene immobilization, influenced the catalyst activity as well as the polymer characteristics. The pore size and its distribution affect the catalyst activity through the formation of bimolecular species and the diffusion of reagents to the catalyst sites. The variation in the Zr–O interatomic distance influences the polymer molecular weight. Increasing this distance engenders polymers with a lower molecular weight.

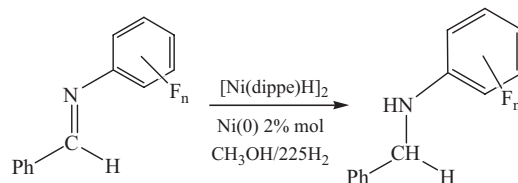


Ana L. Iglesias, Juventino J. García

Journal of Molecular Catalysis A: Chemical 298 (2009) 51

Homogeneous hydrogenation of fluoroaromatic imines with Ni compounds, evidence for η^2 -C=N intermediate in the catalytic cycle

The hydrogenation of fluorinated imines with Ni compounds was achieved. High conversions to their corresponding amines were obtained using polar donor solvents such as methanol. Although transfer hydrogenation of imines is observed, H_2 pressure is needed to drive the reaction to completion. Evidences for the η^2 -C=N coordination as a first step of a catalytic cycle is presented.

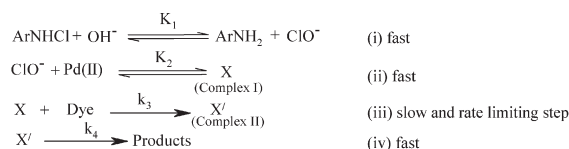


K.N. Vinod, Puttaswamy, K.N. Ninge Gowda

Journal of Molecular Catalysis A: Chemical 298 (2009) 60

Oxidative decolorization of triphenylmethane dyes by chloramine-T in alkaline medium catalyzed by Pd(II): A comparative spectrophotometric kinetic and mechanistic approach

The kinetics of oxidative decolorization of p-rosaniline, crystal violet and ethyl violet dyes by chloramine-T (CAT or ArNHCl) in presence of NaOH and Pd(II) catalyst were studied spectrophotometrically at 303 K. Reactions in all the three dyes followed the identical kinetics and the below scheme is proposed for the reaction.



Above scheme leads to the following rate law,

$$\text{rate} = \frac{K_1 K_2 k_3 [\text{CAT}]_t [\text{Dye}] [\text{OH}^-] [\text{Pd(II)}]}{[\text{ArNH}_2] + K_1 [\text{OH}^-] + K_1 K_2 [\text{OH}^-] [\text{Pd(II)}]}$$

Above scheme leads to the following rate law,

$$\text{rate} = \frac{K_1 K_2 K_3 [\text{CAT}]_t [\text{Dye}] [\text{OH}^-] [\text{Pd(II)}]}{[\text{ArNH}_2] + K_1 [\text{OH}^-] + K_1 K_2 [\text{OH}^-] [\text{Pd(II)}]}$$

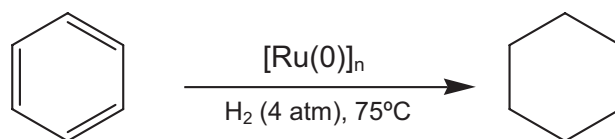
The proposed scheme and the derived rate law are in good agreement with the observed kinetic data.

Liane M. Rossi, Giovanna Machado

Journal of Molecular Catalysis A: Chemical 298 (2009) 69

Ruthenium nanoparticles prepared from ruthenium dioxide precursor: Highly active catalyst for hydrogenation of arenes under mild conditions

Ru(0) nanoparticles prepared by a very simple method based on the reduction of the commercially available precursor ruthenium dioxide under mild condition are highly active catalysts for the hydrogenation of benzene. At 75 °C and 4 atm hydrogen pressure, we obtained total turnovers of 2700 and 1200 mol/mol Ru in solventless and ionic liquid biphasic conditions, respectively.

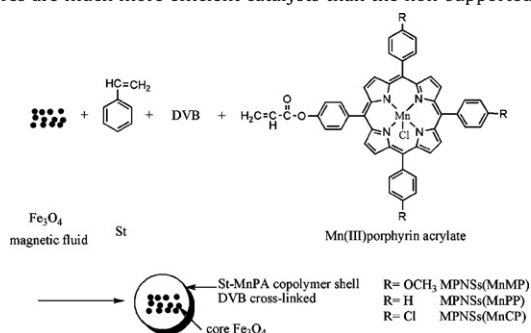


Bo Fu, Han-Cheng Yu, Jin-Wang Huang, Ping Zhao, Jie Liu, Liang-Nian Ji

Journal of Molecular Catalysis A: Chemical 298 (2009) 74

Mn(III) porphyrins immobilized on magnetic polymer nanospheres as biomimetic catalysts hydroxylating cyclohexane with molecular oxygen

Three types of magnetic polymer nanospheres immobilizing Mn(III) porphyrins with different phenyl substituents were synthesized and their catalytic activities to hydroxylate cyclohexane with molecular oxygen were investigated. These magnetic nanospheres are much more efficient catalysts than the non-supported Mn(III) porphyrin analogues and can be completely recovered and efficiently reused.

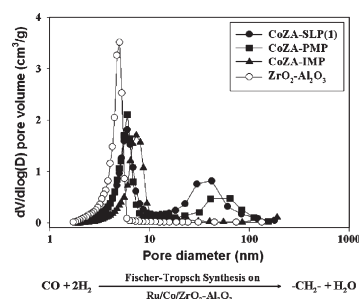


Seon-Ju Park, Jong Wook Bae, Jong-Hyeok Oh, K.V.R. Chary, P.S. Sai Prasad, Ki-Won Jun, Young-Woo Rhee

Journal of Molecular Catalysis A: Chemical 298 (2009) 81

Influence of bimodal pore size distribution of Ru/Co/ZrO₂-Al₂O₃ during Fischer-Tropsch synthesis in fixed-bed and slurry reactor

The Ru/Co/ZrO₂-Al₂O₃ (CoZA) catalysts were prepared by slurry precipitation (SLP) and conventional impregnation method to investigate their catalytic performance during Fischer-Tropsch synthesis. The CoZA-SLP, possessing a bimodal pore size distribution with the homogeneously distributed cobalt clusters, showed high catalytic performances due to the high mass-transfer efficiency and small cobalt cluster size of around 10 nm.

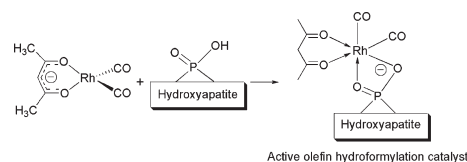


Kun Wang, Gordon J. Kennedy, Raymond A. Cook

Journal of Molecular Catalysis A: Chemical 298 (2009) 88

Hydroxyapatite-supported Rh(CO)₂(acac) (acac = acetylacetonate): Structure characterization and catalysis for 1-hexene hydroformylation

Supporting Rh(CO)₂(acac) (acac = acetylacetonate) on hydroxyapatite Ca₁₀(PO₄)₆(OH)₂ gives an active catalyst for 1-hexene hydroformylation without the presence of an auxiliary ligand such as phosphine.

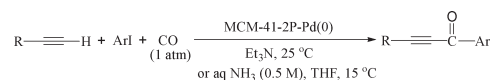


Wenyan Hao, Junchao Sha, Shouri Sheng, Mingzhong Cai

Journal of Molecular Catalysis A: Chemical 298 (2009) 94

The first heterogeneous carbonylative Sonogashira coupling reaction catalyzed by MCM-41-supported bidentate phosphine palladium(0) complex

The first heterogeneous carbonylative Sonogashira coupling reaction of terminal alkynes with aryl iodides under atmospheric pressure of CO was achieved in the presence of a catalytic amount of MCM-41-supported bidentate phosphine palladium(0) complex. This polymeric palladium catalyst can be reused at least 10 times without any decrease in activity.

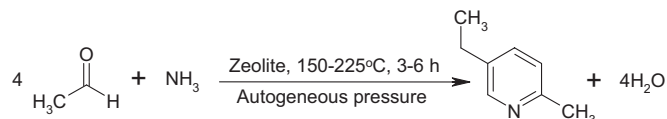


K.V.V. Krishna Mohan, K. Suresh Kumar Reddy, N. Narender, S.J. Kulkarni

Journal of Molecular Catalysis A: Chemical 298 (2009) 99

Zeolite catalysed synthesis of 5-ethyl-2-methylpyridine under high pressure

Simple and selective single-step synthesis of 5-ethyl-2-methylpyridine (EMP) under high pressure (autogeneous pressure) conditions is achieved with high conversion and high selectivity over zeolites. The catalyst can be reused many times without significant loss of activity.

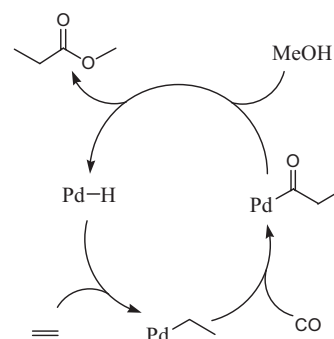


E. Amadio, G. Cavinato, A. Dolmella, L. Ronchin, L. Toniolo, A. Vavasori

Journal of Molecular Catalysis A: Chemical 298 (2009) 103

New carboalkoxybis(triphenylphosphine) palladium (II) cationic complexes: Synthesis, characterization, reactivity and role in the catalytic hydrocarboalkoxylation of ethene. X-ray structure of *trans*-[Pd(COOMe)(TsO)(PPh₃)₂]-2CHCl₃

The new cationic complexes *trans*-[Pd(COOR)(H₂O)(PPh₃)₂](TsO (R = Me, Et, *n*-Pr, *iso*-Pr, *n*-Bu, *iso*-Bu, *sec*-Bu)) have been synthesised and characterised by IR, ¹H NMR and ³¹P NMR spectroscopies. The structure of *trans*-[Pd(COOMe)(TsO)(PPh₃)₂]-2CHCl₃ has been determined by X-ray diffraction studies. The reactivity of the carbomethoxy complex with alkanols, TsOH/H₂O and ethene has been studied in relation with the catalytic hydrocarboalkoxylation of the olefin. All the carboalkoxy complexes are catalyst precursors for the carboalkoxylation of ethene if used in the combination of PPh₃ and TsOH, better in the presence of some water. Experimental evidences are more in favor of the so-called "hydride" mechanism rather than the "carbomethoxy" mechanism.

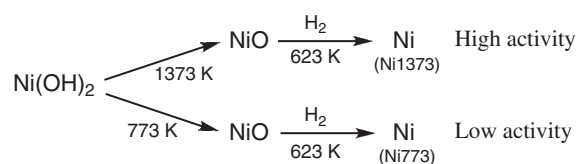


Tsutomu Osawa, Yuki Hamano, Sachiyo Saga, Osamu Takayasu

Journal of Molecular Catalysis A: Chemical 298 (2009) 111

Hydrogen–deuterium exchange of methane on nickel surface prepared by the reduction of nickel oxide

The hydrogen–deuterium exchange reactions of methane in a deuterium stream were studied over a reduced nickel catalyst. The reduced nickel (Ni1373) prepared from nickel oxide calcined at 1373 K had a higher activity than the reduced nickel (Ni773) prepared from the nickel oxide calcined at 773 K. As the Ni1373 could predominantly have a Ni(1 0 0) surface, Ni1373 had a higher activity than Ni773.



Jui-Ying Tsai, Jiunn-Hsing Chao, Chiu-Hsun Lin

Journal of Molecular Catalysis A: Chemical 298 (2009) 115

Low temperature carbon monoxide oxidation over gold nanoparticles supported on sodium titanate nanotubes

Small gold particles having sizes of 1.0–2.0 nm were deposited on the sodium trititanate nanotube (Na₂Ti₃O₇) surface by the ion exchange method. The gold catalyst with a loading of 2.53 wt.% Au could achieve a T_{50%} of 218 K in a pulse reactor with a reactant pulse containing 0.34 μmol CO/pulse.

