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Contents

Articles

Zhicheng Zhang, Shangtao Chen, Xiaofan Zhang, Huayi Li, Yucai Ke, Yingying Lu, Youliang Hu

Journal of Molecular Catalysis A: Chemical 230 (2005) 1

A series of novel 2,6-bis(imino)pyridyl iron catalysts: synthesis, characterization and ethylene oligomerization A series of 2,6-bis(imino)pyridyl iron complexes have been synthesized and used for oligomerization of ethylene. These complexes, activated with methylaluminoxane (MAO), lead to highly active ethylene oligomerization (> 10^7 g/molFeh) and most products are linear α -olefins (>90%). Steric and electronic effects due to different substituents at aryl rings on catalytic activities and distributions of oligomers are studied.

Bassam El Ali, Jimoh Tijani, Mohammed Fettouhi

Journal of Molecular Catalysis A: Chemical 230 (2005) 9

Selective hydroformylation–acetalization of arylalkenes in methanol catalyzed by $RhCl_3 \cdot 3H_2O-P(OPh)_3$ system

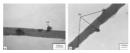
The regioselective hydroformylation–acetalization of alkenes can be achieved in one-pot reaction in the presence of $RhCl_3 \cdot 3H_2O$ as a catalysts and triphenylphosphite $[P(OPh)_3]$ as a ligand in pure methanol as a solvent. The reaction with styrene was carried out at $80^{\circ}C$ and 600psi ($CO/H_2=1/1$) to produce the branched acetal and the linear acetals as the major products (B/L=92/8). The total yield of this reaction was 90%. $RhCl_3 \cdot 3H_2O$ showed the highest catalytic activity compared to other rhodium catalysts use in this process. The effects of the type of the catalyst, co-catalyst and the type of alcohol have been studied.

Huaping Liu, Guoan Cheng, Ruiting Zheng, Yong Zhao, Changlin Liang

Journal of Molecular Catalysis A: Chemical 230 (2005) 17

Influence of acid treatments of carbon nanotube precursors on Ni/CNT in the synthesis of carbon nanotubes

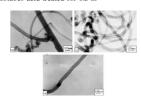
The Ni catalysts supported on the carbon nanotubes acid-treated for 0.5 and 6h were successfully prepared by directly dipping the carbon nanotube precursors refluxed in dilute nitric acid into Ni electroless plating bath. And the mean Ni particle size and the metal-support contact area were smaller when the carbon nanotubes precursors were acid-treated for 6h.



Bamboo-shaped carbon nanotubes and Y junction carbon nanotubes were synthesized with Ni catalyst supported on carbon nanotubes acid-treated for $0.5\ h$ in dilute nitric acid.



The carbon nanotubes with high quality were synthesized with Ni supported on carbon nanotubes acid-treated for 6 h in dilute nitric acid, indicating that this kind of catalyst show higher activity in the synthesis of new carbon nanotubes than Ni catalyst supported on carbon nanotubes acid-treated for $0.5\,h$.



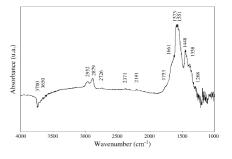
vi Contents

J.L. Valverde, A. de Lucas, F. Dorado, A. Romero, P.B. García

Journal of Molecular Catalysis A: Chemical 230 (2005) 23

Study by in situ FTIR of the SCR of NO by propene on Cu^{2+} ion-exchanged Ti-PILC

In situ IR study of SCR of NO by propene showed that reaction intermediates were mainly NO_3^- species, C_3H_7 – NO_2 and acetate. Cu^{2+} –OH groups reacted with the nitro group, thus forming nitrate.



Gianluca Melillo, Lorella Izzo, Roberto Centore, Angela Tuzi, Alexander Z. Voskoboynikov, Leone Oliva

Journal of Molecular Catalysis A: Chemical 230 (2005) 29

meso-Me₂Si(1-indenyl)₂ZrCl₂/methylalumoxane catalyzed polymerization of the ethylene to ethylbranched polyethylene

With the title catalyst polyethylene with large amount of branching and low molecular weight can be obtained, possibly as a consequence of the high rate of β -H transfer.

$$CH_2CH_2$$

MAO

M. Jhansi L. Kishore, G.S. Mishra, Anil Kumar

Journal of Molecular Catalysis A: Chemical 230 (2005) 35

Synthesis of hetero binuclear macrocyclic CoV complex bonded to chemically modified alumina support for oxidation of cyclohexane using oxygen

A binuclear macrocyclic complex $Co^{II}V^{IV}L^{2+}$ bonded to carbamate-modified alumina is used as a catalyst for oxidation of cyclohexane. The catalyst was thermally stable up to $251^{\circ}C$. The products formed were cyclohexanone and cyclohexanol without any isomerization or cracking products.

Shin-ichiro Fujita, Bhalchandra M. Bhanage, Hiroshi Kanamaru, Masahiko Arai

Journal of Molecular Catalysis A: Chemical 230 (2005) 43

Synthesis of 1,3-dialkylurea from ethylene carbonate and amine using calcium oxide

CaO has been found to be an excellent recyclable catalyst for the synthesis of dialkylureas from ethylene carbonate (EC) and amines. Dialkylureas are obtained under mild conditions with high yields. Propylene carbonate can be used instead of EC for the reaction. A plausible reaction mechanism is proposed.

$$0 \\ O \\ O \\ + 2RNH_2 \\ \hline CaO$$

$$R \\ N \\ H \\ H$$

$$R \\ + HO$$

$$OH$$

Contents vii

Yoshihiko Ohishi, Tomonori Kawabata, Tetsuya Shishido, Ken Takaki, Qinghong Zhang, Ye Wang, Katsuomi Takehira

Journal of Molecular Catalysis A: Chemical 230 (2005) 49

Dehydrogenation of ethylbenzene with CO_2 over Cr-MCM-41 catalyst

G. Kumaraswamy, Nivedita Jena, M.N.V. Sastry, G. Venkata Rao, K. Ankamma

Journal of Molecular Catalysis A: Chemical 230 (2005) 59

Synthesis of 6,6'- and 6-MeO-PEG-BINOL-Ca soluble polymer bound ligands and their application in asymmetric Michael and epoxidation reactions

The first synthesis of enantioenriched Ca-bound soluble polymer BINOL ligand for the activation of asymmetric Michael addition and epoxidation reactions. This monometallic catalyst works not only as a Lewis acid but also as a Bronsted base.

Ge Luo, Shirun Yan, Minghua Qiao, Kangnian Fan

Journal of Molecular Catalysis A: Chemical 230 (2005) 69

Effect of promoters on the structures and properties of the RuB/ γ -Al₂O₃ catalyst

Effect of promoters (Co, Fe, Sn, Zn) on structures, properties and catalytic performance of RuB/ γ -Al₂O₃ catalyst was studied using in situ XRD, TEM, H₂-TPD, XPS and liquid-phase hydrogenation of ethyl lactate to 1,2-propanediol (PDO).

Éva Balogh-Hergovich, Gábor Speier

Journal of Molecular Catalysis A: Chemical 230 (2005) 79

Catalytic oxidation of alcohols to carbonyl compounds with hydrogen peroxide using dinuclear iron complexes Rapid and efficient oxidation of primary and secondary alcohols was achieved with hydrogen peroxide in acetone in the presence of $[Fe(ind)Cl]_2O$ and $[Fe_2(OMe)_2(PAP)Cl_4]$ as catalysts. The reaction conditions for the oxidation of benzyl alcohol to benzaldehyde with $[Fe(ind)Cl]_2O$ have been optimized by investigating the solvent, type of the oxidant, alcohol/oxidant molar ratio and length of reaction time.

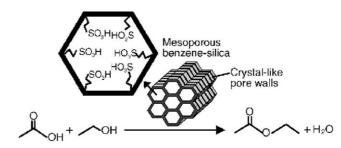
viii Contents

Qihua Yang, Mahendra P. Kapoor, Shinji Inagaki, Nao Shirokura, Junko N. Kondo, Kazunari Domen

Journal of Molecular Catalysis A: Chemical 230 (2005) 85

Catalytic application of sulfonic acid functionalized mesoporous benzene-silica with crystal-like pore wall structure in esterification

Excellent catalytic activity in esterification of acetic acid with ethanol is achieved on sulfonic acid functionalized mesoporous benzene-silica with crystal-like periodic pore walls.



György Szöllősi, Shu-Ichi Niwa, Taka-Aki Hanaoka, Fujio Mizukami

Journal of Molecular Catalysis A: Chemical 230 (2005) 91

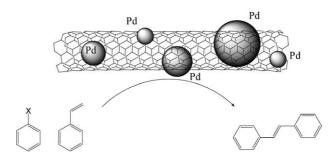
Enantioselective hydrogenation of α,β -unsaturated carboxylic acids over cinchonidine-modified Pd catalysts: effect of substrate structure on the adsorption mode

The preferential adsorption of α,β -unsaturated carboxylic acids during their enantioselective hydrogenation over cinchonidine-modified Pd catalysts is directed by the nature of the substituent (alkyl or aryl) situated in β position.

Avelino Corma, Hermenegildo Garcia, Antonio Leyva

Journal of Molecular Catalysis A: Chemical 230 (2005) 97

Catalytic activity of palladium supported on single wall carbon nanotubes compared to palladium supported on activated carbon. Study of the Heck and Suzuki couplings, aerobic alcohol oxidation and selective hydrogenation Palladium nanoparticles spontaneously generated by contacting Pd(OAc)₂ with single wall carbon nanotubes are more active for the Suzuki and Heck coupling reaction than palladium supported on activated carbon.



J.S. Yadav, A.V. Narsaiah, B.V.S. Reddy, A.K. Basak, K. Nagaiah

Journal of Molecular Catalysis A: Chemical 230 (2005) 107

Niobium(V) chloride: an efficient catalyst for selective acetylation of alcohols and phenols

Contents ix

Biju M. Devassy, G.V. Shanbhag, F. Lefebvre, Walter Böhringer, Jack Fletcher, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 230 (2005) 113

Zirconia-supported phosphotungstic acid as catalyst for alkylation of phenol with benzyl alcohol

Liquid phase alkylation of phenol with benzyl alcohol using zirconia supported phosphotungstic acid as catalyst was investigated and 15% PTA on zirconia calcined at 750°C gave 98% benzyl alcohol conversion with 83% benzyl phenol selectivity at optimized conditions.

OH
$$_{+}$$
 $_{+}$ $_{+}$ $_{+}$ $_{+}$ $_{+}$ $_{+}$ $_{+}$ $_{-}$

Yong Ding, Baochun Ma, Qiang Gao, Guixian Li, Liang Yan, Jishuan Suo

Journal of Molecular Catalysis A: Chemical 230 (2005) 121

A spectroscopic study on the 12-heteropolyacids of molybdenum and tungsten (H_3PMo_{12} – $_nW_nO_{40}$) combined with cetylpyridinium bromide in the epoxidation of cyclopentene

The epoxidation of cyclopentene with hydrogen peroxide catalyzed by $H_3PMo_6W_6O_{40}$ combined with cetylpyridinium bromide as a phase transfer reagent was carried out in acetonitrile. The fresh catalysts and the catalysts under reaction condition were characterized by UV–vis, FT-IR and ^{31}P NMR spectroscopies, which have revealed that all of the molybdotungstophosphoric acids were degraded in the presence of hydrogen peroxide to form a considerable amount of phosphorus-containing species. The active species resulted from $H_3PMo_6W_6O_{40}$ are new kinds of phosphorus-containing species, which is different from $\{PO_4[WO(O_2)_2]_4\}^{3-}$.

$$\frac{H_{3}PMo_{6}W_{6}O_{40} + CPB}{H_{2}O_{2} + CH_{3}CN}$$

Ying Xiao, Sanjay V. Malhotra

Journal of Molecular Catalysis A: Chemical 230 (2005) 129

Friedel-Crafts alkylation reactions in pyridiniumbased ionic liquids The Friedel–Crafts alkylations of benzene in pyridinium-based ionic liquids (ILs) were investigated. Reactions were found to proceed under mild conditions with excellent conversion. The ILs could be recycled and reused without a significant change in product conversion, as opposed to traditional solvent–catalyst systems.

IL: $[EtPy]^{\dagger}[CF_3COO]^{\dagger}$ or $[EtPy]^{\dagger}[BF_4]^{\dagger}$

Fei Peng, Jun Ling, Zhiquan Shen, Weiwei Zhu

Journal of Molecular Catalysis A: Chemical 230 (2005) 135

Correlation between phenol structure and catalytic activity of samarium(III) phenolates in polymerization of ϵ -caprolactone. Part 2. Tertbutyl's electronic and steric effects

Six novel single component catalysts, Sm(III) phenolates, for the ring-opening polymerization of ϵ -caprolactone were synthesized The experimental results were discussed together with quantum chemical (QC) calculation data describing the phenols' geometric and charge distribution parameters in organized groups. Tertbutyls' electronic and steric effects on phenolates' catalytic activity and ROP characteristics were found with both experimental and calculational support.



x Contents

Lingping Wang, Aiguo Kong, Bo Chen, Hanming Ding, Yongkui Shan, Mingyuan He

Journal of Molecular Catalysis A: Chemical 230 (2005) 143

Direct synthesis, characterization of Cu-SBA-15 and its high catalytic activity in hydroxylation of phenol by $\rm H_2O_2$

Transition metals copper substituted mesoporous silica Cu-SBA-15 has firstly been obtained. The Cu(II) ion was mainly incorporated into the framework of Cu-SBA-15 forming a new type active site which raises the phenol conversion to 62.4% and diphenol selectivity to 97.2% in phenol hydroxylation.

Ajayan Vinu, Mani Karthik, Masahiko Miyahara, Velayudam Murugesan, Katsuhiko Ariga

Journal of Molecular Catalysis A: Chemical 230 (2005) 151

ortho-Selective ethylation of phenol with ethanol catalyzed by bimetallic mesoporous catalyst, CoAl-MCM-41

Ethylation of phenol with ethanol was studied in vapor-phase using CoAl-MCM-41 catalysts. The *C*-alkylation is dominant, and more than 90% of the products can be assigned the *C*-alkylated ethyl phenols under the selected condition. Preferential *ortho*-substitution occurred probably to the proximity effect between small ethyl cation and *ortho*-position of phenol on the catalyst surface.

