



Journal of Molecular Catalysis A: Chemical 208 (2004) 1-10

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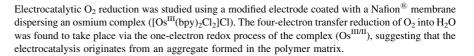
Contents

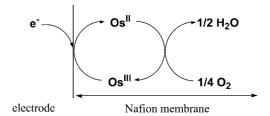
Articles

Toshiyuki Abe, Kuniaki Shoji, Akio Tajiri

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Electrocatalysis of molecular aggregate composed of an osmium complex and a polymer membrane for dioxygen reduction



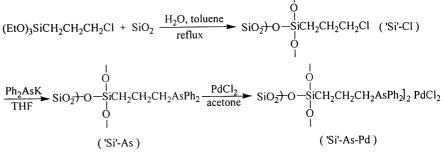


Mingzhong Cai, Yizheng Huang, Ronghua Hu, Caisheng Song

The synthesis of a silica-supported poly- γ -diphenylarsinopropylsiloxane palladium complex has been described. This polymeric palladium complex is an efficient catalyst for Heck carbonylation of aryl halides and can be recovered and reused.

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Synthesis of silica-supported poly- γ -diphenylarsinopropylsiloxane palladium complex and its catalytic behavior for Heck carbonylation of aryl halides



V.B. Valodkar, G.L. Tembe, M. Ravindranathan, R.N. Ram, H.S. Rama

Journal of Molecular Catalysis A: Chemical 208 (2004) 21

 $Catalytic \ oxidation \ by \ polymer-supported \ copper(II)-L-valine \ complexes$

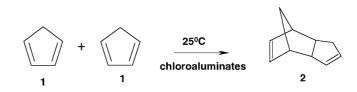
L-Valine was anchored to 6 and 8% cross-linked poly(styrene-divinyl benzene) resin and its complex with copper acetate was prepared. The polymer-supported Cu complexes behave as versatile and recyclable catalysts for the oxidation of benzyl alcohol, cyclohexanol and styrene. The influence of different reaction parameters on conversion and selectivity to products are reported.

$$C_6H_5$$
-CH₂OH C_6H_5 -CH₂OH C_6H_5 -CHO

Anil Kumar, Sanjay S. Pawar

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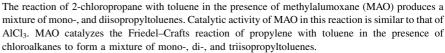
AlCl₃-catalysed dimerization of 1,3-cyclopentadiene in the chloroaluminate room temperature ionic liquid

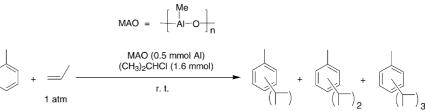


Junpei Kuwabara, Daisuke Takeuchi, Kohtaro Osakada

Journal of Molecular Catalysis A: Chemical 208 chloro (2004) 39

MAO-catalyzed Friedel-Crafts reactions of toluene with chloroalkanes and with propylene



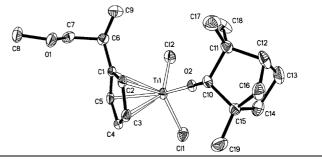


Yanlong Qian, Hao Zhang, Junxia Zhou, Wei Zhao, Xueqin Sun, Jiling Huang

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Synthesis and polymerization behavior of various substituted half-sandwich titanium complexes Cp'TiCl₂(OR*) as catalysts for syndiotactic polystyrene

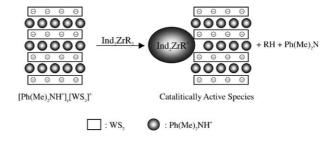
A new set of chiral alkoxyl substituted half-sandwich titanium complexes of $Cp'TiCl_2(OR^*)$ were synthesized, characterized and tested as catalyst precursors for the syndiospecific polymerization of styrene. The structure of complex **8** was confirmed by X-ray diffraction. The effects of variation on temperature, Al/Ti ratio for catalytic activity and Syndiotactic polystyrene (s-PS%) were also studied.



Satoru Yamada, Akihiro Yano, Morihiko Sato, Takahito Itoh

Journal of Molecular Catalysis A: Chemical 208 (2004) 55

Effect of "topotactic" reduction product of tungsten disulfide on catalytic activity of metallocene catalyst for olefin polymerization Addition of *N*,*N*-dimethylanilinium ion (Ph(Me)₂NH⁺) intercalated WS₂ as a cocatalyst to Ind₂ZrCl₂/Et₃Al was found to improve significantly the catalytic activity for ethylene polymerization. It was proposed that neutral dialkylmetallocene was protonated by Ph(Me)₂NH⁺ in the interlayer space of WS₂, especially on the surface of the cocatalyst, to form the cationic monoalkylmetallocene and that the two-dimensional macroanion of WS₂ functioned as a non-coordinating anion and a carrier for the cationic species.



2

P.J. Baricelli, L. Izaguirre, J. López, E. Lujano, Francisco López-Linares

Journal of Molecular Catalysis A: Chemical 208 (2004) 67

Synthesis, characterization and catalytic hydrogenation in aqueous-biphasic system of a new water soluble complex RuH(CO)(NCMe) $(TPPMS)_3[BF_4]$

In this work, we are reporting the synthesis, characterization and preliminaries catalytic studies of the new hydrosoluble ruthenium complex [RuH(CO)(CH₃CN)(TFFMS)₃]BF₄, during the biphasic hydrogenation reaction of 1-hexene and cyclohexene. The hydrosoluble complex was active in the hydrogenation of 1-hexene and cyclohexene under the following reaction conditions: $T = 80^{\circ}$ C, P = 400 psi of hydrogen, S/C ratio = 100:1 and water/heptane = 1:1. Under this reaction conditions, only the corresponding saturated product is obtained without evidence of isomerization products.

> RuHCl(CO)(TFFMS)₃+NaBF₄+CH₃CN→RuH(CO)(CH₃CN)TFFMS)₃B F,+NaCl TPPMS TPPMS NCCH/

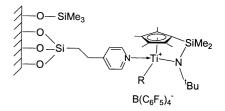
TPPMS

Kittichote Musikabhumma, Thomas P. Spaniol, Jun Okuda

Journal of Molecular Catalysis A: Chemical 208 (2004) 73

Tritylpyridinium tetrakis(pentafluorophenyl)borate as an efficient activator for "constrainedgeometry" catalysts in ethylene polymerization

Ethylene polymerization by linked amido-cyclopentadienyl or "constrained-geometry" titanium catalysts, $Ti(\eta^5:\eta^1-C_5Me_4SiMe_2N^tBu)X_2$ (X = Me, Bz, Cl) was found to proceed with high activity when activated with tritylpyridinium tetrakis(pentafluorophenyl)borate, $[Ph_3C(C_5H_5)]$ $[B(C_6F_5)_4]$. The silica-supported tritylpyridinium tetrakis(entafluorophenyl)borate (PySTB) also produced high molecular weight polyethylenes with excellent morphology and high bulk density.

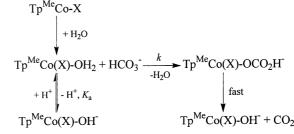


Ying-Ji Sun, Lei Z. Zhang, Peng Cheng, Hua-Kuan Lin, Shi-Ping Yan, Dai-Zheng Liao, Zong-Hui Jiang, Pan-Wen Shen

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Experimental and theoretical studies of the dehydration kinetics of two inhibitor-containing halfsandwich cobalt(II) complexes

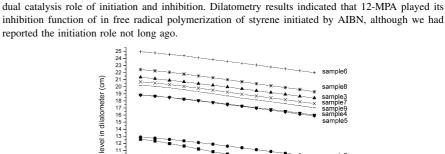
The dehydration kinetic measurements of HCO₃⁻ catalyzed by two inhibitor-containing half-sandwich cobalt(II) complexes have been performed by the stopped-flow techniques. Results from this work indicate that the five-coordinated aqua complex must be the reactive catalytic species in the catalyzed dehydration reaction and the rate-determining step is the substitution of the labile water molecule by HCO₃⁻.



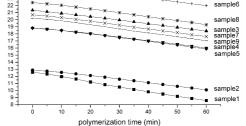
Dianyu Chen, Zhigang Xue, Zhixing Su

Journal of Molecular Catalysis A: Chemical 208 (2004) 91

Dual role study of 12-molybdophosphoric acid on styrene polymerization



12-Molybdophosphoric acid (12-MPA) was studied in present paper as a special polymeried catalyst with

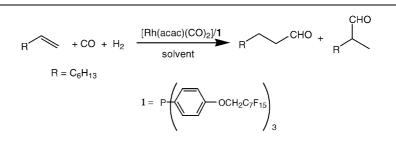


Contents

Ali Aghmiz, Carmen Claver, Anna M. Masdeu-Bultó, David Maillard, Denis Sinou

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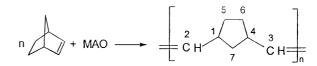
Hydroformylation of 1-octene with rhodium catalysts in fluorous systems



Valia Amir-Ebrahimi, John J. Rooney

Journal of Molecular Catalysis A: Chemical 208 (2004) 103

Methylaluminoxane as a novel catalyst and cocatalyst for ring-opening metathesis polymerisation of norbornene



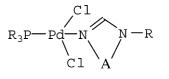
Methylaluminoxane (MAO) alone catalyses the ring-opening metathesis polymerisation of norbornene. It is also a very effective cocatalyst when used with various Mo and W compounds for this reaction, giving

İsmail Özdemir, Bekir Çetinkaya, Serpil Demir

Journal of Molecular Catalysis A: Chemical 208 (2004) 109

Synthesis of novel 1-alkylimidazoline and 1-alkylbenzimidazole palladium(II) complexes as efficient catalysts for Heck and Suzuki reactions involving arylchlorides The synthesis and characterization of the new palladium(II) complexes of the type $[PdCl_2(PR_3)L]$, (L = 1-alkyl-2-imidazoline or 1-alkylbenzimidazole) have been prepared. *N*-coordinated complexes of palladium(II) gave high catalytic activity in the Suzuki coupling and Heck reaction of aryl halides.

very stereo-blocky polymers.



$$A = CH_2CH_2$$
 or C_6H_4

Valia Amir-Ebrahimi, John J. Rooney

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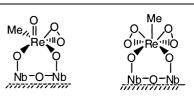
Remarkable alternating effect in metathesis copolymerization of norbornene and cyclopentene using modified Grubbs ruthenium initiators When the Grubbs initiator, $RuCl_2(PCy_3)_2$ (=CHPh), is used with $MoCl_5$ in dry dichloromethane as solvent, but not in ethers, to catalyse the metathesis of mixtures of norbornene and cyclopentene, a strongly alternating copolymer is formed. The use of WCl_6 in place of $MoCl_5$ moderates the catalyst more severely such that almost only homopolymer of cyclopentene is obtained. These results are attributed to cage formation that greatly reduces access of the more bulky norbornene to the metallacarbene.

$$n + n + n + n + MoCl_2 (PCy_3)_2 (= CHPh) + MoCl_5 + MoCl_5$$

Ming Li, James H. Espenson

Journal of Molecular Catalysis A: Chemical 208 (2004) 123

Kinetic study of epoxidations by urea-hydrogen peroxide catalyzed by methyltrioxorhenium(VII) on niobia Relative rates were measured by competition kinetics for concurrent, heterogeneous epoxidations of olefins with urea–hydrogen peroxide (UHP) in CDCl₃ catalyzed by MeReO₃ on Nb₂O₅.

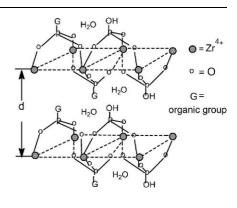


Catalytically active intermediates

Ma Xuebing, Fu Xiangkai

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Synthesis of the novel layered amorphous and crystalline zirconium phosphate–phosphonates Zr(HPO₄)[O₃PCH₂N(CH₂CH₂)₂O]·*n*H₂O, Zr(HPO₄)[O₃PCH₂N(CH₂CO₂H)₂]·*n*H₂O, zirconium phosphonates Zr[(O₃PCH₂)NCH₂CO₂H] ·*n*H₂O and the catalytic activities of their palladium complexes in hydrogenation The layered amorphous and crystalline samples of Zr(HPO₄)[O₃PCH₂N(CH₂CH₂)₂O]·nH₂O (1a, 2a). Zr(HPO₄)[O₃PCH₂N(CH₂CO₂H)₂]·nH₂O (1b, 2b) and Zr[(O₃PCH₂)₂NCH₂CO₂H]·nH₂O (1c, 2c) were synthesized for the first time. The samples were comparatively characterized by XRD, IR, TG and elemental analysis. XRD data showed that the crystalline samples 2a, 2b and 2c are highly crystalline with interlayer spacings of 1.606, 1.538 and 1.239 nm respectively. Their palladium complexes possessed good activities in the hydrogenation of carbon-corbon double bond. The catalytic activities of the palladium complexes of amorphous 1a, 1b and 1c is 1.5-3.1 times as high as that of the palladium complexes of crystalline 2a, 2b and 2c.

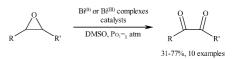


Sylvain Antoniotti, Elisabet Duñach

Journal of Molecular Catalysis A: Chemical 208 (2004) 135

Studies on the catalytic oxidation of epoxides to α -diketones by Bi⁽⁰⁾/O₂ in DMSO

Catalytic oxidation of internal epoxides by bismuth derivatives under molecular oxygen in DMSO affords the corresponding α -diketones. The influence of several parameters such as of the nature of the catalyst, Bi^(III) salts or Bi⁽⁰⁾, the solvent, the presence of additives and other oxidants has been examined. The preparation of a series of linear and cyclic, aliphatic and aromatic α -diketones is reported in 31–77% yields.

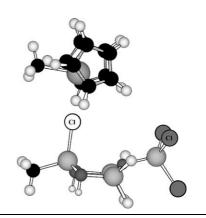


P.G. Belelli, D.E. Damiani, N.J. Castellani

Journal of Molecular Catalysis A: Chemical 208 (2004) 147

Effect of a Lewis acid additive on active sites formation in zirconocene catalyst systems: a DFT study

The interaction of Cp_2ZrCl_2/MAO catalytic system and AlCl₃ was studied theoretically. The stabilities of different ionic-pairs were considered and analyzed from the electronic structure point of view.



Zaihui Fu, Dulin Yin, Qingji Xie, Wei Zhao, Aixia Lv, Donghong Yin, Youzhi Xu, Luxi Zhang

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Ti complexes assembled HMS as effective catalysts for epoxidation of alkene

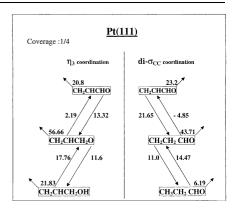
Ti tartrate complex $(Ti(O'Pr)_4 + DET)$ -grafted hexagonal mesoporous silica (HMS) catalysts have been successfully prepared through three assembled pathways, and show the high catalytic activity and a definite epoxidative enantioselectivity for the epoxidation of styrene with tetrabutyl hydroperoxide (TBHP) as an oxidant.

 $PhCH=CH_{2} \underbrace{HMS-Ti(OiPr)_{4}-DET}_{2(CH_{3})_{3}C-OOH(TBHP)} PhCHO + PhCH_{2}CHO + \frac{H_{1}}{H} \underbrace{C - C}_{H} + \frac{H_{1}}{H} \underbrace{C$

B.C. Khanra, Y. Jugnet, J.C. Bertolini

Journal of Molecular Catalysis A: Chemical 208 (2004) 167

Energetics of acrolein hydrogenation on $Pt(1 \ 1 \ 1)$ and $Ag(1 \ 1 \ 1)$ surfaces: a BOC-MP model study Activation barriers for hydrogenation of acrolein to allyl alcohol and propanal on Pt(111) and Ag(111) surfaces are estimated by bond-order conservation-Morse potential (BOC-MP) model. A comparison of the barriers explains the lower selectivity for allyl alcohol compared to that for propanal.

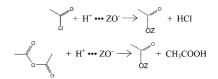


O. Kresnawahjuesa, R.J. Gorte, David White

Journal of Molecular Catalysis A: Chemical 208 (2004) 175

Characterization of acylating intermediates formed on H-ZSM-5

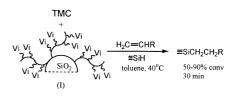
Acetyl-zeolite intermediate is formed below 400K when typical Friedel-Craft acylating agents such as acetyl chloride and acetic anhydride reacted with Brønsted-acid site of H-ZSM-5.



Z.M. Michalska, Ł. Rogalski, K. Rózga-Wijas, J. Chojnowski, W. Fortuniak, M. Ścibiorek

Journal of Molecular Catalysis A: Chemical 208 (2004) 187

Synthesis and catalytic activity of the transition metal complex catalysts supported on the branched functionalized polysiloxanes grafted on silica Hybrid supports (I) prepared by grafting on silica vinyl-functionalized linear and branched polysiloxanes were used for immobilizing the transition metal complexes, TMC (Pt, Rh). These heterogenized catalysts effectively catalyzed hydrosilylation of terminal alkene. The catalyst activity was found to be dependent on the type of a parent complex, the degree of branching and the content of the vinyl ligands.



Contents

Si⁴⁺, Al³⁺
Al³⁺, Mg²⁺

OH

Claudia Crestini, Alessandra Pastorini, Pietro Tagliatesta

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Metalloporphyrins immobilized on motmorillonite as biomimetic catalysts in the oxidation of lignin model compounds *meso*-Tetrakis(tetramethylpyridinio)porphyrin pentaacetate immobilized on the smectite clay montmorillonite is an efficient biomimetic catalyst for hydrogen peroxide oxidation of lignin model compounds.

Hiroshi Kanzaki, Takahiro Kitamura,

Journal of Molecular Catalysis A: Chemical 208

Activities for phenol formation using Cu catalysts supported on Al_2O_3 in the liquid-phase oxidation of benzene in aqueous solvent with high acetic

Rei Hamada, Satoru Nishiyama,

Shigeru Tsuruya

acid concentration

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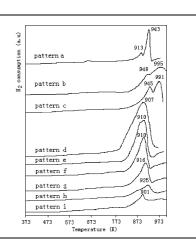
Huachang Jiang, Weimin Lu, Huilin Wan

Journal of Molecular Catalysis A: Chemical 208 (2004) 213

The effect of $MoV_{0.3}Te_{0.23}P_xO_n$ catalysts with different phosphorus content for selective oxidation of propane to acrolein

The effect of $MoV_{0.3}Te_{0.23}P_xO_n$ catalysts with different phosphorus content for selective oxidation of propane to acrolein and with XRD and TPR characterization.

acid.

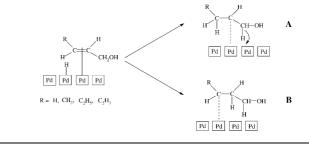


M.G. Musolino, P. De Maio, A. Donato, R. Pietropaolo

Journal of Molecular Catalysis A: Chemical 208 (2004) 219

Hydrogenation versus isomerization in α , β -unsaturated alcohols reactions over Pd/TiO₂ catalysts

Hydrogenation and isomerization of α,β -unsaturated alcohols have been investigated in tetrahydrofuran over Pd/TiO₂ catalysts at 303K and 0.01MPa partial hydrogen pressure. The double bond isomerization reaction of these substrates affords also the corresponding saturated aldehydes or ketones. Catalytic activity and selectivity depend strongly on the steric and electronic effects characteristic of the organic substrate. A mechanism involving two σ -alkyl palladium bonded intermediates was proposed.



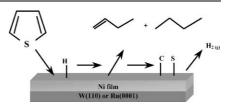
Contents

Neetha A. Khan, Jingguang G. Chen

Journal of Molecular Catalysis A: Chemical 208 (2004) 225

Thiophene HDS chemistry on monolayer Ni films on $W(1\ 1\ 0)$ and $Ru(0\ 0\ 0\ 1)$

In this paper, we have shown thiophene chemistry on surfaces covered with monolayer Ni films. Adding Ni to the closed-packed surfaces of W and Ru alters the HDS activity of these surfaces at temperatures below 300K, and the resulting reactivity is unlike either pure metal. However, above 1ML Ni, the Ni/W(110) and Ni/Ru(0001) surfaces begin to act like Ni surfaces.



Rick B. Watson, Shannon L. Lashbrook, Umit S. Ozkan

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Chlorine modification of Mo/silica-titania mixedoxide catalysts for the oxidative dehydrogenation of ethane

C. Constantin, V. Pârvulescu, A. Bujor, G. Popescu, B.L. Su

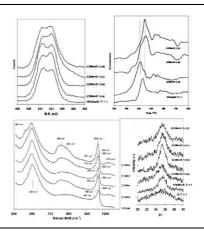
Journal of Molecular Catalysis A: Chemical 208 (2004) 245

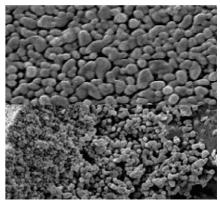
Mesoporous nickelsilicate membranes on porous alumina supports

I. Effect of nature and surface pretreatment of alumina supports on the catalytic membrane formation

A series of molybdenum-based catalysts have been prepared and studied in regard to their performance in the oxidative dehydrogenation (ODH) of ethane. The effect of alkali (K and Li) and halide (Cl⁻) modifiers on catalyst performance has been evaluated by doping at a low level (dopant/ Mo molar ratio = 0.1). The changes in reaction performance are related to the nature of the supported MoO_x surface species that are significantly affected by the introduction of chlorine. While the addition of halide modifiers is known to positively affect the gas-phase mechanisms of ethane ODH at higher temperatures (>650°C), current work indicates that the effect for surface redox mechanisms over MoO_x-based catalysts may be somewhat lesspronounced, but still beneficial, at lower temperatures of operation.

Ordered mesoporous nickelsilicate catalytic membranes have been synthesized on the surface of γ alumina disk and α -alumina tube by dip coating and immersion and intensively characterized. Their permeation and separation properties have been evaluated and correlated with nature of alumina supports, their surface treatment and conditions of the hydrothermal synthesis.





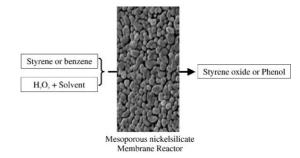
V. Pârvulescu, C. Constantin, G. Popescu, B.L. Su

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Mesoporous nickelsilicate membranes on porous alumina supports

II. Catalytic reactor for oxidation of aromatic hydrocarbons

The catalytic properties of nickelsilicate membranes have been evaluated in the reaction of styrene and benzene with H_2O_2 and compared with powdery catalyst in the batch reactor. The significant difference in selectivity was noted that membrane gave styrene oxide as only and final product while batch reactor led to the formation of deeper oxidation product: benzaldehyde.

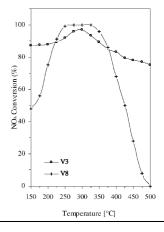


S. Djerad, L. Tifouti, M. Crocoll, W. Weisweiler

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Effect of vanadia and tungsten loadings on the physical and chemical characteristics of V_2O_5 - WO_3/TiO_2 catalysts

The selective catalytic reduction of NO_x by ammonia over 3%V₂O₅--9%WO₃/TiO₂ and 8%V₂O₅--9%WO₃/TiO₂ catalyst prepared by the sol-gel method have been investigated. More significant changes in activity occurs on the catalyst V8 which displayed a higher NO_x conversion but in a narrow temperature range while V3 exhibits a lower reactivity but with high selectivity to N₂ over the whole temperature range.

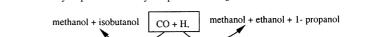


Daiping He, Yunjie Ding, Hongyuan Luo, Can Li

 ZrO_2 -based catalyst is found to be an effective catalyst in the synthesis of ethanol or isobutanol, and their selectivities basically depend on the crystal phase of ZrO_2 surface.

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Effects of zirconia phase on the synthesis of higher alcohols over zirconia and modified zirconia





Natalia V. Semagina, Alexei V. Bykov, Esther M. Sulman, Valentina G. Matveeva, Stanislav N. Sidorov, Lidia V. Dubrovina, Peter M. Valetsky, Olga I. Kiselyova, Alexei R. Khokhlov, Barry Stein, Lyudmila M. Bronstein

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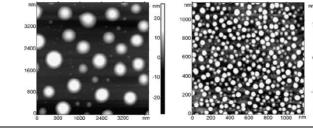
Selective dehydrolinalool hydrogenation with poly(ethylene oxide)-*block*-poly-2-vinylpyridine micelles filled with Pd nanoparticles

Carlos Carone, Viviane de Lima, Fernanda Albuquerque, Paula Nunes, Cristóvão de Lemos, João H.Z. dos Santos, Griselda B. Galland, Fernanda C. Stedile, Sandra Einloft, Nara R. de S. Basso

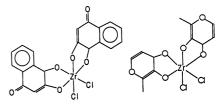
Journal of Molecular Catalysis A: Chemical 208 (2004) 285

Zirconium alkoxide complexes as catalysts for ethylene polymerization

Dehydrolinalool (3,7-dimethyloct-6-ene-1-yne-3-ol, DHL) hydrogenation to linalool (3,7-dimethylocta-1,6-diene-3-ol, LN) was studied with Pd nanoparticles formed in poly(ethylene oxide)-*block*-poly-2vinylpyridine (PEO-*b*-P2VP) micelles varying micelle characteristics by varying the solvent composition and pH of the reaction medium. The larger and denser the micelles (left), the slower the reaction, while selectivity reaches 99.4%. High reaction rates were observed for small micelles (right). The highest TOF achieved is 24.4s⁻¹.

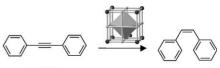


The synthesis and catalytic activity of two zirconium complexes bearing 2-hydroxy-1,4-naphthoquinone and 3-hydroxy-2-methyl-4-pyrone as ligands is reported. Both catalysts were also grafted on silica and on methylaluminoxane (MAO)-modified silica and evaluated in ethylene polymerization.



Stefan Kaskel, Klaus Schlichte, Tobias Kratzke

Journal of Molecular Catalysis A: Chemical 208 (2004) 291 Titanium nitride nanoparticles show a high catalytic activity and selectivity in hydroalumination reactions.



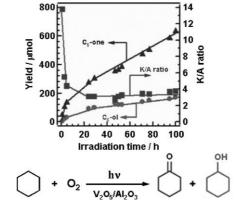


Catalytic properties of high surface area titanium nitride materials

Kentaro Teramura, Tsunehiro Tanaka, Masaya Kani, Tomohiro Hosokawa, Takuzo Funabiki

Journal of Molecular Catalysis A: Chemical 208 (2004) 299

Selective photo-oxidation of neat cyclohexane in the liquid phase over V_2O_5/Al_2O_3



András Fási, István Pálinkó, Ágnes Gömöry, Imre Kiricsi

Journal of Molecular Catalysis A: Chemical 208 (2004) 307

Ring opening, dimerisation and oligomerisation reactions of methyloxirane on solid acid and base catalysts

Methyloxirane undergoes a variety of reactions over catalysts of widely differing acid–base characteristics. Single ring opening, cyclic dimerisation and linear oligomerisation all occur on the nearly superacidic Nafion-H, while single ring opening is predominant over the basic Mg–Al hydrotalcite. The behaviour of K10 montmorillonite and NaN₃-loaded SiMCM-41 are in-between of the two extremes.

