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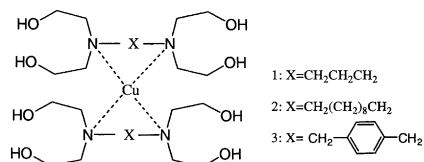
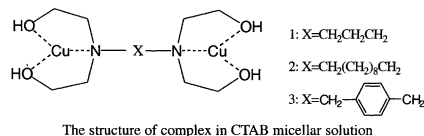
Articles

**Jiang Fubin, Jiang Bingying, Chen Yong,
Yu Xiaoqi, Zeng Xiancheng**

*Journal of Molecular Catalysis A: Chemical 210
(2004) 9*

Metallomicellar catalysis: effects of bridge-connecting ligands on the hydrolysis of PNPP catalyzed by Cu(II) complexes of ethoxyl-diamine ligands in micellar solution

In the catalytic hydrolysis of PNPP, the kinetically active species has been determined to be the 2:1 (metal:ligand) complex in CTAB micellar solution, in contrast, to the 1:2 (metal:ligand) complex of the ligand to Cu²⁺ in Brij35 micellar solution.

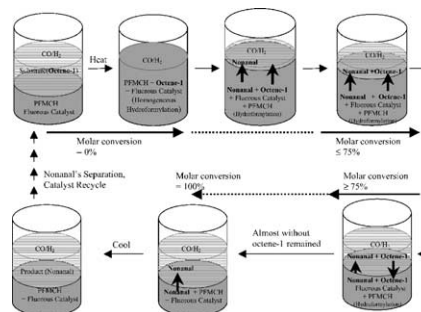


**Yulin Huang, Evangelia Perperi,
George Manos, David J. Cole-Hamilton**

*Journal of Molecular Catalysis A: Chemical 210
(2004) 17*

Performance of octene in fluoruous biphasic hydroformylation: octene distribution and reversible transfer between perfluoromethylcyclohexane and nonanal

During fluoruous biphasic hydroformylation 1-octene is transferred from the fluoruous into the organic product phase and then from the product layer back to the fluoruous layer again, due to the immiscibility of nonanal with PFMCH. The effect of the temperature and the total amount of octene on the above behaviour were also studied.

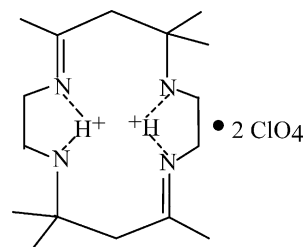


**Xingming Kou, Siqing Cheng, Juan Du,
Xiaoqi Yu, Xiancheng Zeng**

*Journal of Molecular Catalysis A: Chemical 210
(2004) 23*

Catalytic hydrolysis of carboxylic acid esters by Cu(II) and Zn(II) complexes containing a tetra-coordinate macrocyclic Schiff base ligand in Brij35 micellar solution

The kinetics and mechanisms for the hydrolysis of two carboxylic esters in Brij35 micellar solution catalyzed by macrocyclic Schiff base complex of Cu(II) and Zn(II) are reported. The differences in mechanisms are highlighted.

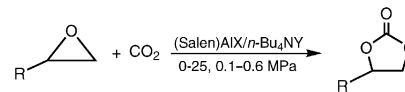


**Xiao-Bing Lu, Ying-Ju Zhang, Bin Liang,
Xiao Li, Hui Wang**

Journal of Molecular Catalysis A: Chemical 210
(2004) 31

Chemical fixation of carbon dioxide to cyclic carbonates under extremely mild conditions with highly active bifunctional catalysts

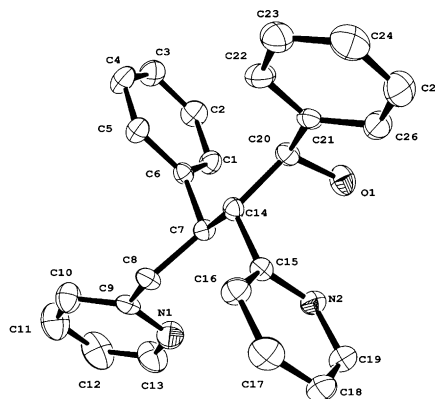
Chemical fixation of CO₂ to cyclic carbonates proceeds effectively under extremely mild temperature and pressure by using a bifunctional nucleophile–electrophile catalyst system.



**Dong Mok Shin, Seung Uk Son, Bog Ki Hong,
Young Keun Chung, Sung-Ho Chun**

Journal of Molecular Catalysis A: Chemical 210
(2004) 35

Preparation of palladium complexes of 1,3-di(2-pyridyl)propane derivatives and their use in norbornene polymerization

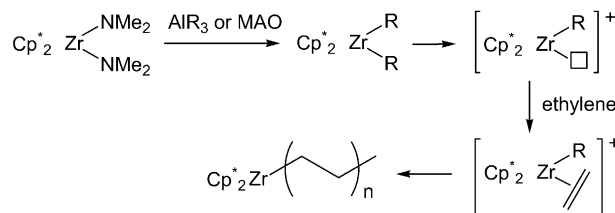


Il Kim, Chang-Sik Ha

Journal of Molecular Catalysis A: Chemical 210
(2004) 47

Polymerization of ethylene with (C₅Me₅)₂Zr(NMe₂)₂ cocatalyzed by common alkyl aluminums

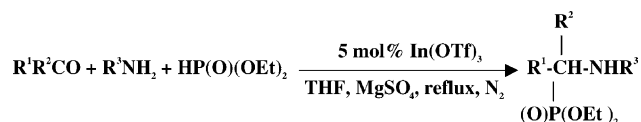
Polymerizations of ethylene by using Cp₂^{*}Zr(NMe₂)₂ (Cp^{*} = C₅Me₅) compound yielded high activity combined with common alkyl aluminums or methylaluminoxane (MAO) as cocatalysts. The catalytic activities obtained by Cp₂^{*}Zr(NMe₂)₂/AlR₃ and Cp₂^{*}Zr(NMe₂)₂/MAO catalysts demonstrate that both MAO and AlR₃ are effective cocatalysts to generate cationic [Cp₂^{*}Zr-R]⁺ active species.



**Rina Ghosh, Swarupananda Maiti,
Arijit Chakraborty, Dilip K. Maiti**

Journal of Molecular Catalysis A: Chemical 210
(2004) 53

In(OTf)₃ catalysed simple one-pot synthesis of α-amino phosphonates

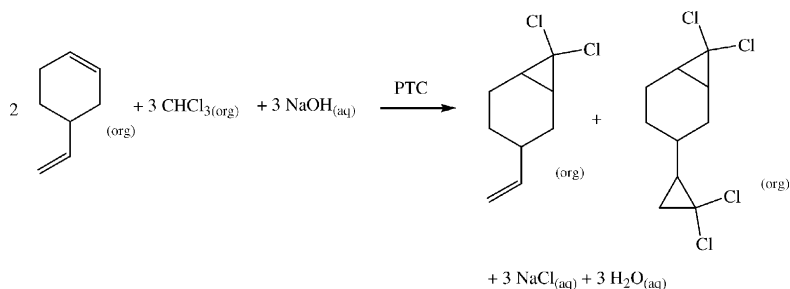


Maw-Ling Wang, Yu-Ming Hsieh

Journal of Molecular Catalysis A: Chemical 210 (2004) 59

Kinetic study of dichlorocyclopropanation of 4-vinyl-1-cyclohexene by a novel multisite phase transfer catalyst

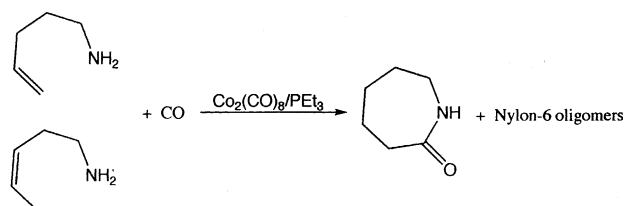
The dichlorocyclopropanation of 4-vinyl-1-cyclohexene (reactant) in an alkaline solution/organic solvent two-phase medium under phase transfer catalysis conditions was carried out to produce 7,7-dichloro-3-vinyl-bicyclo[4.1.0]heptane (mono-adduct) and 7,7-dichloro-3-(2,2-dichloro-cyclopropyl)-bicyclo[4.1.0]heptane (di-adduct).

**Shengsheng Liu, Ayusman Sen, Rudy Parton**

Journal of Molecular Catalysis A: Chemical 210 (2004) 69

Cobalt-catalyzed synthesis of ϵ -caprolactam and nylon-6 from aminopentene and carbon monoxide

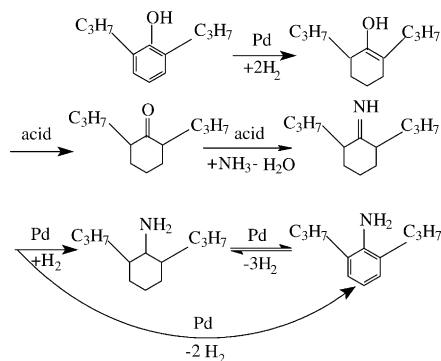
ϵ -Caprolactam and nylon-6 oligomers were synthesized from 4-pentene-1-amine and/or 3-pentene-1-amine and carbon monoxide using a catalyst system consisting of $\text{Co}_2(\text{CO})_8$ and excess PEt_3 .

**Ruixia Jiang, Zaiku Xie, Chengfang Zhang, Qingling Chen**

Journal of Molecular Catalysis A: Chemical 210 (2004) 79

GC-MS analysis and reaction mechanism of the gas-phase amination of 2,6-diisopropylphenol

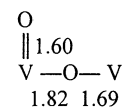
The liquid product of the gas-phase amination of 2,6-diisopropylphenol (2,6-DIPP) to prepare 2,6-diisopropylaniline (2,6-DIPA) was analyzed using gas chromatography-mass spectrometry. The reaction mechanism of gas-phase amination of 2,6-DIPP on the bifunctional palladium-lanthanum supported catalyst was proposed. This reaction was synergistically catalyzed by the Pd metal active sites and the acid sites on the catalyst support.

**A. Klisińska, A. Haras, K. Samson, M. Witko, B. Grzybowska**

Journal of Molecular Catalysis A: Chemical 210 (2004) 87

Effect of additives on properties of vanadia-based catalysts for oxidative dehydrogenation of propane. Experimental and quantum chemical studies

DFT calculations for VO_xA cluster where A: K, P, Ni, Cr, Mo, show good agreement between the extent of electron transfer from A to VO_x and propene selectivity in propane oxidative dehydrogenation (ODH), determined experimentally for $\text{VO}_x\text{A}/\text{SiO}_2$ (VSiA) catalysts.

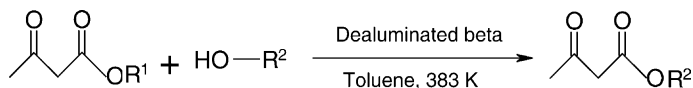


M. Sasidharan, R. Kumar

Journal of Molecular Catalysis A: Chemical 210 (2004) 93

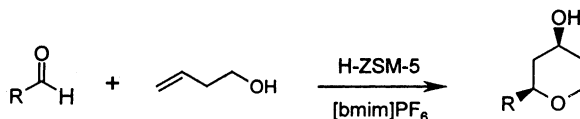
Transesterification over various zeolites under liquid-phase conditions

Transesterification of β -keto esters with a variety of alcohols over aluminosilicates was accomplished simply by refluxing in toluene under liquid-phase conditions. Large-pore zeolites such as Y, MOR, and BEA show higher activity than the medium-pore ZSM-5 and the partial removal of framework aluminum from the large-pore zeolites by dealumination increases their activity.

**J.S. Yadav, B.V.S. Reddy, M. Sridhar Reddy, N. Niranjana**

Journal of Molecular Catalysis A: Chemical 210 (2004) 99

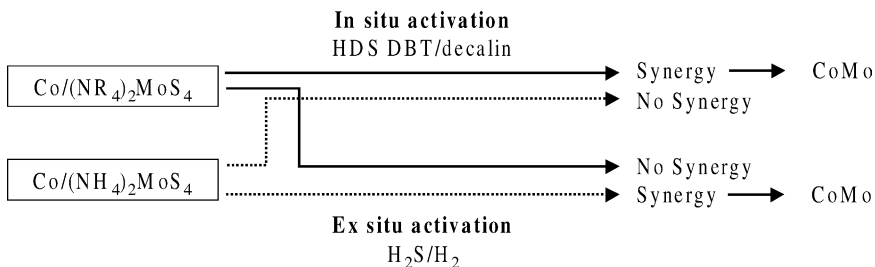
Eco-friendly heterogeneous solid acids as novel and recyclable catalysts in ionic medium for tetrahydropyrans

**L. Alvarez, J. Espino, C. Ornelas, J.L. Rico, M.T. Cortez, G. Berhault, G. Alonso**

Journal of Molecular Catalysis A: Chemical 210 (2004) 105

Comparative study of MoS_2 and Co/MoS_2 catalysts prepared by ex situ/in situ activation of ammonium and tetraalkylammonium thiomolybdates

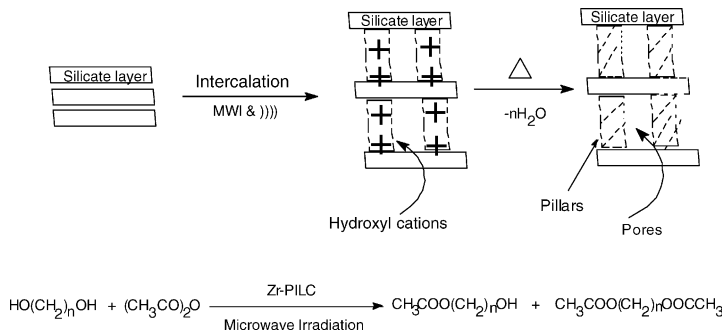
Ammonium and tetraalkylammonium thiomolybdates $(\text{NR}_4)_2\text{MoS}_4$ (R: H, methyl, propyl) were used to synthesize MoS_2 and CoMo catalysts. Two types of activation were performed: an ex situ activation under a $\text{H}_2\text{S}/\text{H}_2$ flow before the hydrodesulfurization of dibenzothiophene or an in situ activation by direct decomposition under HDS conditions. For in situ activated catalysts, the cobalt synergistic effect is enhanced by the presence of carbon in the precursor.

**Vasundhara Singh, Varinder Sapehiya, Goverdhan Lal Kad**

Journal of Molecular Catalysis A: Chemical 210 (2004) 119

Ultrasound and microwave activated preparation of ZrO_2 -pillared clay composite: catalytic activity for selective, solventless acylation of 1,n-diols

The successful preparation of ZrO_2 -pillared clay composite by a new and efficient strategy employing ultrasonication in conjunction with microwave heating is reported. It is catalytically active for the selective mono-acylation of symmetrical 1,n-diols in solventless conditions under microwave irradiation.

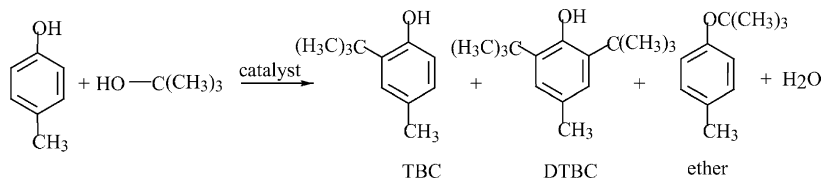


Biju M. Devassy, G.V. Shanbhag, F. Lefebvre, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 210 (2004) 125

Alkylation of *p*-cresol with *tert*-butanol catalyzed by heteropoly acid supported on zirconia catalyst

Butylation of *p*-cresol by *tert*-butanol was catalyzed by 12-tungstophosphoric acid supported on zirconia. Fifteen percent TPA/ZrO₂ was the most active catalyst in butylation of *p*-cresol under optimized reaction conditions 403K, Bu/Cr molar ratio 3 and LHSV 4h⁻¹ with conversion *p*-cresol (61mol%) and total butylated product selectivity (99.5%). The catalyst tested for 100h showed only 6% loss in the catalytic activity in terms of conversion of *p*-cresol.

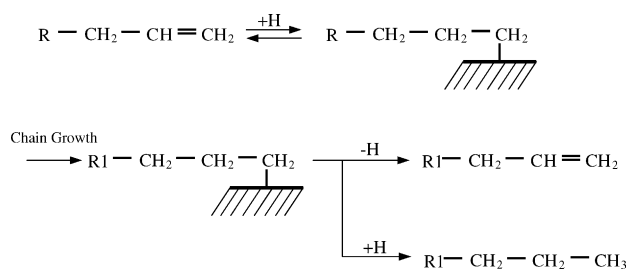


Sung-Chul Lee, Jea-Hun Jang, Byung-Yong Lee, Jun-Sik Kim, Misook Kang, Sang-Bong Lee, Myung-Jae Choi, Suk-Jin Choung

Journal of Molecular Catalysis A: Chemical 210 (2004) 131

Promotion of hydrocarbon selectivity in CO₂ hydrogenation by Ru component

Once formed linear α -olefins can readsorb on the catalyst surface and undergo secondary reactions: hydrogenation, isomerization, re-insertion, hydrogenolysis and hydroformylation. They can re-adsorb and form an alkyl chain attached to the catalyst surface. This surface species can again either grow further or desorb as an olefin or a paraffin, the latter reaction thereby leading to hydrogenation of the readsorbed olefin. Therefore, the readsorption of α -olefin products played a critical role in hydrocarbon chain growth.

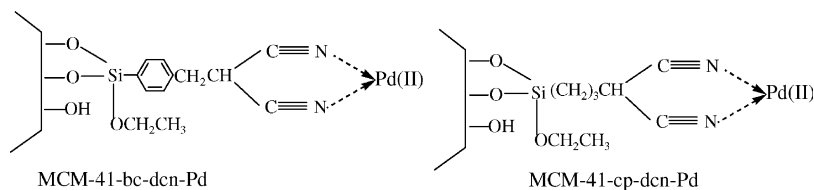


Hengquan Yang, Gaoyong Zhang, Xinlin Hong, Yinyan Zhu

Journal of Molecular Catalysis A: Chemical 210 (2004) 143

Dicyano-functionalized MCM-41 anchored-palladium complexes as recoverable catalysts for Heck reaction

Palladium were anchored on dicyano-functionalized MCM-41 prepared by surface modification, resulting in new heterogeneous catalysts for Heck reaction. The developed catalysts demonstrated easy separation and good reusability.

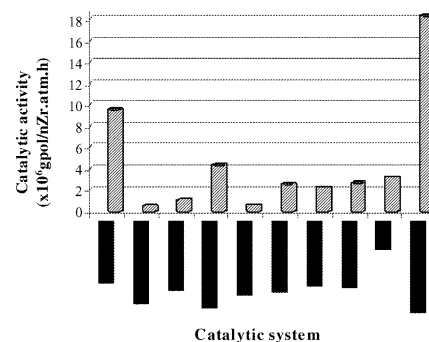


Griselda Barrera Galland, João H.Z. dos Santos, Fernanda C. Stedile, Paula Palmeira Greco, Adriano D. Campani

Journal of Molecular Catalysis A: Chemical 210 (2004) 149

Ethylene homo- and copolymerization using (*n*BuCp)₂ZrCl₂ grafted on silica modified with different spacers

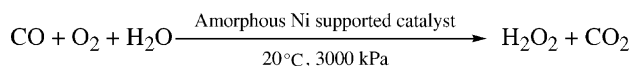
(*n*BuCp)₂ZrCl₂ was grafted on silica modified by polymethylhydrosiloxane (PMHS), Me₃SiCl, Ph₃SiOH, SnCl₄, isodrin and aldrin and evaluated in ethylene/1-hexene copolymerization. The different catalyst systems were compared with the homogenous system and with that resulting from its immobilization on bare silica. (*n*BuCp)₂ZrCl₂ grafted on PMHS-modified silica afforded the catalyst with the highest activity. Comonomer incorporation, melting point and polydispersity was shown to be dependent on the catalyst nature. Bimodality was observed in the case of ethylene homopolymerization employing PMHS-silica-based catalysts.



Zhong-Long Ma, Rong-Li Jia, Chang-Jun Liu*Journal of Molecular Catalysis A: Chemical* 210 (2004) 157

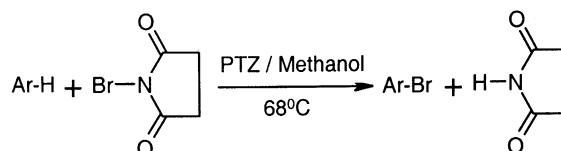
Production of hydrogen peroxide from carbon monoxide, water and oxygen over alumina-supported Ni catalysts

Novel amorphous Ni–B catalysts supported on alumina have been developed for the production of hydrogen peroxide from carbon monoxide, water and oxygen. The experimental investigation confirmed that the promoter/Ni ratio and the preparation conditions have a significant effect on the activity and catalytic lifetime. Among all the catalysts tested, the Ni–La–B/Al₂O₃ catalyst with 1:15 atomic ratio of La/Ni, dried at 120°C, shows the best activity and lifetime for the production of hydrogen peroxide.

**R. Rajagopal, S.A. Siddiqui, Thomas Daniel, R.J. Lahoti, K.V. Srinivasan***Journal of Molecular Catalysis A: Chemical* 210 (2004) 165

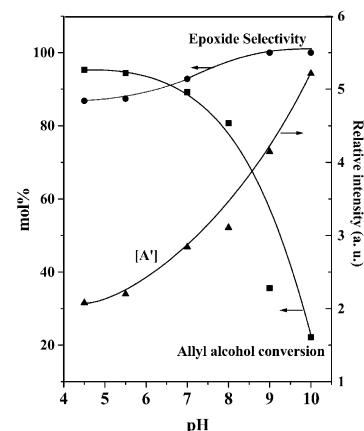
Regioselective side-chain as well as nuclear monobromination of aromatic substrates with *N*-bromosuccinimide using phosphotungstic acid supported on zirconia as a heterogeneous catalyst

Regioselective monobromination of aromatic substrates with *N*-bromosuccinimide has been achieved in excellent isolated yields using phosphotungstic acid supported on zirconia as a novel heterogeneous catalyst. Remarkably, the new catalyst system described brought about the side-chain bromination of aromatics to afford bromomethyl arenes in excellent isolated yields without need for a radical initiator.

**Vasudev N. Shetti, D. Srinivas, P. Ratnasamy***Journal of Molecular Catalysis A: Chemical* 210 (2004) 171

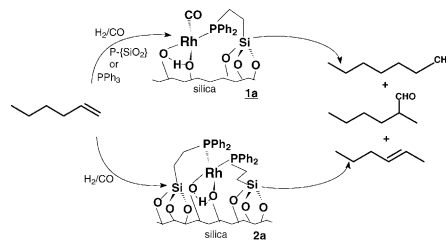
Enhancement of chemoselectivity in epoxidation reactions over TS-1 catalysts by alkali and alkaline metal ions

Alkali metal ions when present during the synthesis of TS-1, lead to inactive oxidation catalysts. However, when added, in small amounts, to the reaction medium during the epoxidation of allyl alcohol or allyl chloride by H₂O₂ over TS-1, they increase the selectivity for the epoxide. This phenomenon is probed, in detail, by investigating the structure and catalytic activities of the oxo-Ti species generated in H₂O₂-TS-1 and TiMCM-41 systems using EPR and diffuse reflectance UV-Vis spectroscopies. Neutralization of surface acidity and modification of Ti sites of TS-1 by alkali ions are probably causes for the enhancement of chemoselectivity.

**Christina M. Standfest-Hauser, Thomas Lummerstorfer, Roland Schmid, Helmuth Hoffmann, Karl Kirchner, Michael Puchberger, Anna M. Trzeciak, Ewa Mieczynska, Włodzimierz Tylus, Józef J. Ziolkowski***Journal of Molecular Catalysis A: Chemical* 210 (2004) 179

Rhodium phosphine complexes immobilized on silica as active catalysts for 1-hexene hydroformylation and arene hydrogenation

Rhodium complexes [Rh(acac)(CO)(Ph₂PCH₂CH₂Si(OMe)₃)] and [Rh(acac)(Ph₂PCH₂CH₂Si(OMe)₃)₂] were immobilized at silica as [Rh(O-{SiO₂})(HO-{SiO₂})(CO)(P-{SiO₂})] (**1a**) and [Rh(O-{SiO₂})(HO-{SiO₂})(P-{SiO₂})₂] (**2a**), respectively, after removal of acac ligands protonated by acidic proton of silica-OH group. Complexes **1a** and **2a** were characterized with ³¹P-CP/MAS, XPS and IR methods and used as pre-catalysts in hydroformylation of 1-hexene. The pre-catalyst **1a** produced up to 54% of aldehydes with Ph₂PCH₂CH₂Si-{SiO₂} co-catalyst and up to 94% with PPh₃ and it was found more active compared to **2a**. Additionally **1a** catalyzes hydrogenation of aromatic hydrocarbons (benzene and toluene).

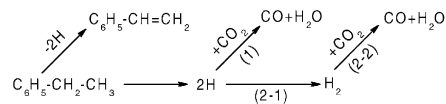


Ailing Sun, Zhangfeng Qin, Shuwei Chen, Jianguo Wang

Journal of Molecular Catalysis A: Chemical 210 (2004) 189

Role of carbon dioxide in the ethylbenzene dehydrogenation coupled with reverse water–gas shift

The role of CO₂ in the ethylbenzene dehydrogenation coupled with the reverse water–gas shift was investigated by means of catalytic reactions, CO₂-TPD as well as thermodynamic analysis.

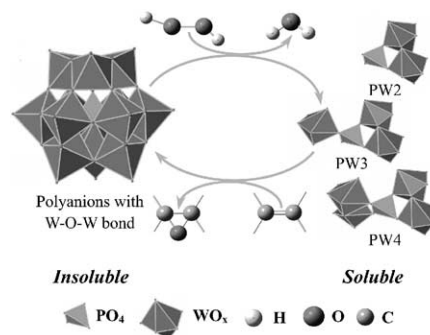


Jinbo Gao, Yangying Chen, Bo Han, Zhaochi Feng, Can Li, Ning Zhou, Shuang Gao, Zuwei Xi

Journal of Molecular Catalysis A: Chemical 210 (2004) 197

A spectroscopic study on the reaction-controlled phase transfer catalyst in the epoxidation of cyclohexene

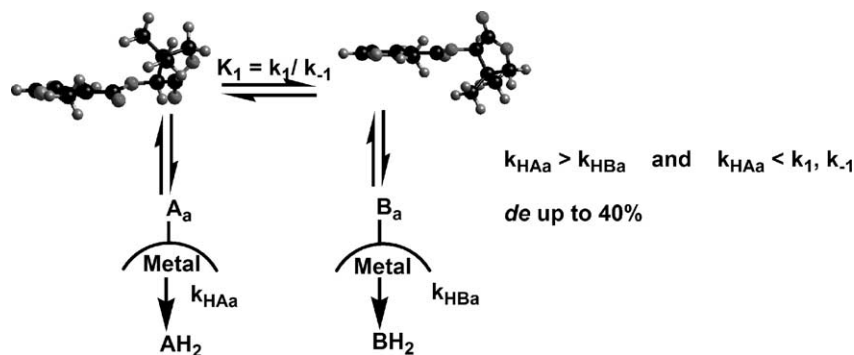
The epoxidation of olefins with hydrogen peroxide in a biphasic medium (H₂O/CHCl₃) was carried out with the reaction-controlled phase transfer catalyst. The catalyst can form smaller soluble active species PW2, PW3, and PW4 via the reaction with hydrogen peroxide. After the hydrogen peroxide is used up, these small anions polymerize into larger anions with forming the W-Ob-W and W-Oc-W bonds, as a result, the catalyst becomes insoluble and precipitates from the reaction medium. The reaction-controlled phase transfer is essentially a process of degradation and polymerization of the catalyst.



Najiba Douja, Raluca Malacea, Michèle Besson, Catherine Pinel

Journal of Molecular Catalysis A: Chemical 210 (2004) 205

Heterogeneous diastereoselective hydrogenation of pyridine and corresponding enamine covalently bound to pantolactone



Olaf Klepel, Cornelia Breitkopf, Mirko Standke

Journal of Molecular Catalysis A: Chemical 210 (2004) 211

Investigation of the aromatization of C₆₊ hydrocarbons on chromia/lanthana-zirconia catalyst. Part I. Catalytic experiments

The aromatization pathway on a chromia/lanthana-zirconia catalyst has been investigated by the conversion of 13 linear and branched hydrocarbons. The product distribution is determined by the educt structure and points to a mechanism without side reactions like isomerization or cracking. The differences in aromatization reactivities could be explained by a mechanism via a stepwise dehydrogenation to a conjugated triene structure.

