

Contents

Articles

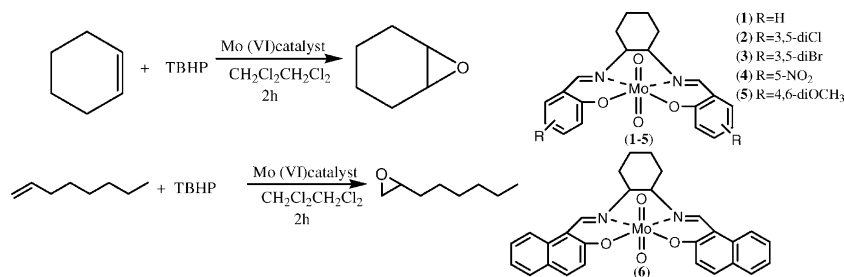
**K. Ambroziak, R. Pelech, E. Milchert,
T. Dziembowska, Z. Rozwadowski**

*Journal of Molecular Catalysis A: Chemical 211
(2004) 9*

New dioxomolybdenum(VI) complexes of tetra-
dentate Schiff base as catalysts for epoxidation of
olefins

Six dioxomolybdenum(VI) complexes of Schiff-base derivatives of *trans*-1,2-diaminocyclohexane and aromatic 2-hydroxyaldehydes were synthesised and employed as selective catalysts in epoxidation of alkenes using *tert*-butyl hydroperoxide as oxidant.

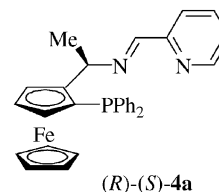
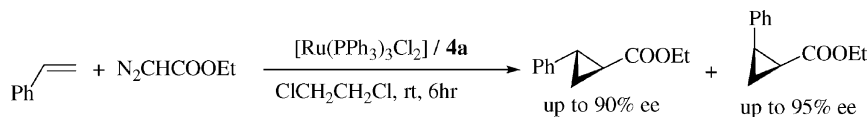
Cyclohexene and 1-octene of rather different reactivity towards epoxidation with hydroperoxides were compared. The effect of temperature and olefin:oxidant molar ratio of the selected catalyst (**5**) on cyclohexene epoxidation were studied.



**Huicong Dai, Xiangping Hu, Huilin Chen,
Changmin Bai, Zhuo Zheng**

*Journal of Molecular Catalysis A: Chemical 211
(2004) 17*

Efficient P,N,N-type ligands for Ru(II)-catalyzed
asymmetric cyclopropanations

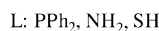
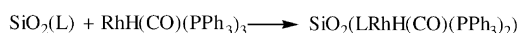
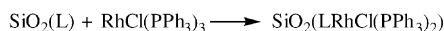
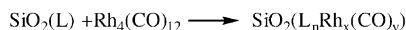


L. Huang, S. Kawi

*Journal of Molecular Catalysis A: Chemical 211
(2004) 23*

Effects of supported donor ligands on the activity
and stability of tethered rhodium complex cata-
lysts for hydroformylation

Three rhodium complexes are tethered to SiO₂ via phosphine, amine and thiol ligands. The aminated SiO₂-tethered catalysts derived from Rh₄(CO)₁₂ and RhCl(PPh₃)₃ display good catalytic activity and good resistance to rhodium leaching. The thiolated SiO₂-tethered catalyst derived from RhH(CO)(PPh₃)₃ exhibits the highest catalytic activity and good resistance to rhodium leaching.

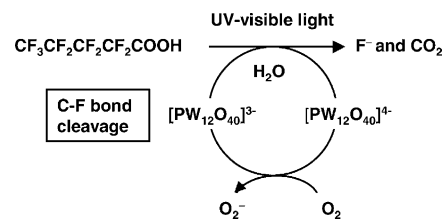


**Hisao Hori, Etsuko Hayakawa,
Kazuhide Koike, Hisahiro Einaga,
Takashi Ibusuki**

Journal of Molecular Catalysis A: Chemical 211 (2004) 35

Decomposition of nonafluoropentanoic acid by heteropolyacid photocatalyst $\text{H}_3\text{PW}_{12}\text{O}_{40}$ in aqueous solution

Nonafluoropentanoic acid can be photocatalytically decomposed to F^- and CO_2 by using water-soluble tungstic heteropolyacid $\text{H}_3\text{PW}_{12}\text{O}_{40}$. The catalytic reaction proceeds under UV-Vis irradiation in water at room temperature and produces no environmentally harmful species, such as CF_4 , which is often observed in the decomposition of perfluorinated compounds by extremely high energy techniques.

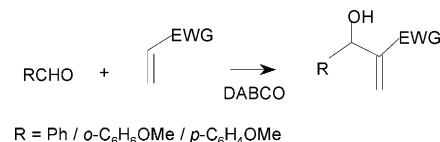


Anil Kumar, Sanjay S. Pawar

Journal of Molecular Catalysis A: Chemical 211 (2004) 43

The DABCO-catalysed Baylis–Hillman reactions in the chloroaluminate room temperature ionic liquids: rate promoting and recyclable media

The DABCO-catalysed Baylis–Hillman reactions are accelerated in the chloroaluminate ionic liquids.

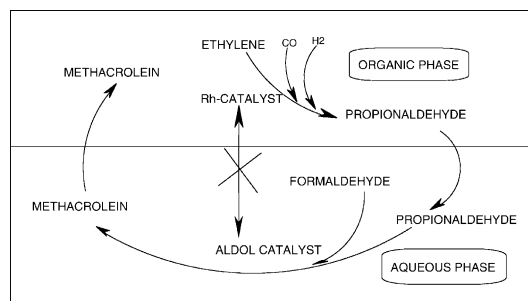


**R.M. Deshpande, M.M. Diwakar,
A.N. Mahajan, R.V. Chaudhari**

Journal of Molecular Catalysis A: Chemical 211 (2004) 49

Biphasic catalysis for a selective oxo–Mannich tandem synthesis of methacrolein

The concept of using different phases for the two catalysts and the products of individual reactions (unique in its application to tandem reactions) ensures an active, selective and stable catalytic system, applied to hydroformylation–aldol sequences. An efficient methacrolein synthesis route via ethylene hydroformylation–aldol condensation with formaldehyde has been proposed.

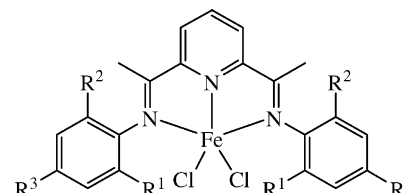


Icaro S. Paulino, Ulf Schuchardt

Journal of Molecular Catalysis A: Chemical 211 (2004) 55

A new iron catalyst for ethylene polymerization

Catalyst **1**, bearing bulky *para*-bromo substituted aryl groups, presents higher catalytic activity than catalyst **2**, giving $4700 \text{ kg PE (mol Fe)}^{-1} \text{ bar}^{-1} \text{ h}^{-1}$ at 20°C , 2 bar of ethylene and an Al/Fe ratio of 1000.



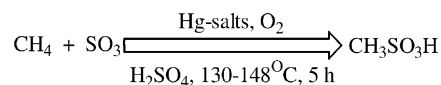
1 $\text{R}^1=\text{R}^2=\text{Me}$; $\text{R}^3=\text{Br}$

2 $\text{R}^1=\text{R}^2=\text{Me}$; $\text{R}^3=\text{H}$

Sudip Mukhopadhyay, Alexis T. Bell

Journal of Molecular Catalysis A: Chemical 211 (2004) 59

Catalyzed sulfonation of methane to methanesulfonic acid

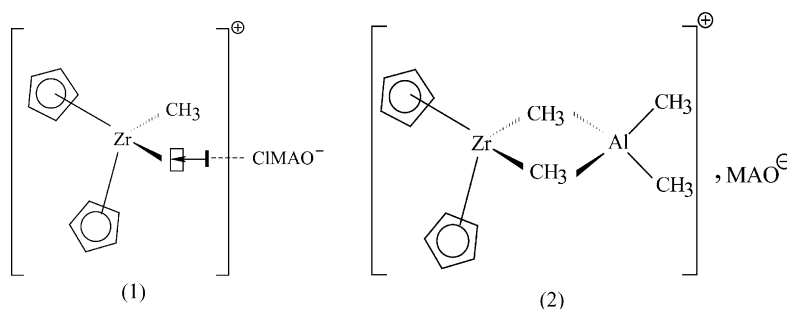


Fábio G. Costa, Lílian M.T. Simplicio, Zênis N. da Rocha, Soraia T. Brandão

Journal of Molecular Catalysis A: Chemical 211 (2004) 67

Study of the catalytic species metallocene/MAO and metallocene/TMA by cyclic voltammetry

An electrochemical study of the metallocene/cocatalyst reaction indicated the formation of the species 1 and 2 formed in MAO and TMA presence, respectively. Both are active in olefin polymerization.

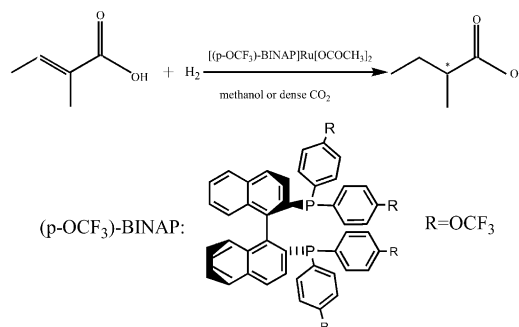


Xing Dong, Can Erkey

Journal of Molecular Catalysis A: Chemical 211 (2004) 73

Enantioselective hydrogenation of tiglic acid in methanol and in dense carbon dioxide catalyzed by a ruthenium-BINAP complex substituted with OCF₃ groups

A fluorinated analog of the ruthenium complex of the 2,2'-bis(diphenylphosphino)-1,1'-binaphthyl (BINAP) ligand was synthesized and tested for hydrogenation of tiglic acid in methanol and dense carbon dioxide.



Dharmesh U. Parmar, Hari C. Bajaj, Raksh V. Jasra, B.M. Moros, V.A. Likholobov

Journal of Molecular Catalysis A: Chemical 211 (2004) 83

Hydroformylation of 1-hexene catalyzed by water soluble CoCl₂(TPPTS)₂ in biphasic medium

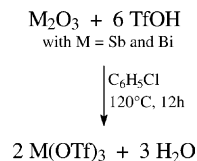
Water soluble cobalt complex of tri(m-sulphophenyl)-phosphine (TPPTS) is found to be selective for aldehyde compared to alcohol during hydroformylation of 1-hexene at 100°C temperature and 9 MPa pressure.

**Magali Peyronneau, Cécile Arrondo,
Laure Vendier, Nicolas Roques,
Christophe Le Roux**

Journal of Molecular Catalysis A: Chemical 211
(2004) 89

An inexpensive and simple process for the preparation of antimony(III) and bismuth(III) triflates

Antimony(III) and bismuth(III) triflates can be prepared quantitatively starting from metal oxides when reacted with a stoichiometric amount of triflic acid in chlorobenzene.

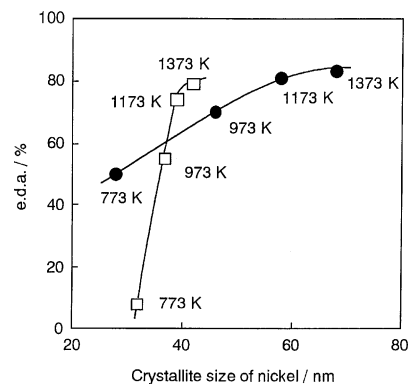


**Tsutomu Osawa, Yuki Amaya, Tadao Harada,
Osamu Takayasu**

Journal of Molecular Catalysis A: Chemical 211
(2004) 93

Enantio-differentiating hydrogenation of methyl acetoacetate over asymmetrically modified reduced nickel catalysts. The effects of the nickel sources on the enantio-differentiating ability

The enantio-differentiating hydrogenation of methyl acetoacetate was carried out over a tartaric acid–NaBr–modified reduced nickel catalyst. Nickel hydroxide and nickel carbonate were used as the precursors of the nickel oxide. They were calcined to nickel oxides, then reduced to nickel metal. It was revealed that the high calcination temperature of the precursors was an important variable for attaining the high enantio-differentiating ability (e.d.a.) of the catalyst.

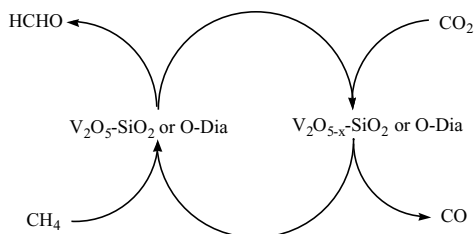


**Takahiro Shimamura, Kimito Okumura,
Kiyoharu Nakagawa, Toshihiro Ando,
Na-oki Ikenga, Toshimitsu Suzuki**

Journal of Molecular Catalysis A: Chemical 211
(2004) 97

Direct formation of formaldehyde from methane and carbon dioxide over vanadium oxide catalysts

Oxidation of CH_4 to HCHO with CO_2 was catalyzed by vanadium oxide loaded on SiO_2 or oxidized diamond (O-Dia) at 873–973K oxygen from CO_2 was supplied to CH_4 via lattice oxygen of vanadium oxide.



**Zhonglai Li, Changhai Liang, Zhaochi Feng,
Pinliang Ying, Dezheng Wang, Can Li**

Journal of Molecular Catalysis A: Chemical 211
(2004) 103

Ammonia synthesis on graphitic-nanofilament supported Ru catalysts

Graphitic-nanofilaments (GNFs) supported ruthenium catalysts were prepared. The Ru particles are in the range of 2–4 nm. The activity of Ru-Ba/GNFs catalysts is higher than that of Ru-Ba/AC by about 25%. The methanation reaction on the Ru/GNFs catalyst is remarkably inhibited compared with a Ru/AC catalyst.



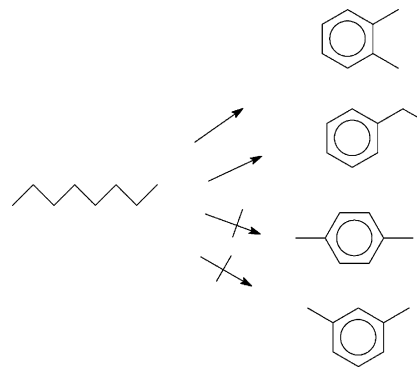
Ru/GNFs catalyst

Cornelia Bretkopf, Olaf Klepel

Journal of Molecular Catalysis A: Chemical 211 (2004) 111

Investigation of the aromatization of C₆₊ hydrocarbons on chromia/lanthana–zirconia catalyst. Part II. Theoretical investigations of stabilities of reactant and intermediate structures

The force field technique and semiempirical calculations with AM1 have been used to calculate stabilities of various linear and branched reactant and product molecules of the aromatization.

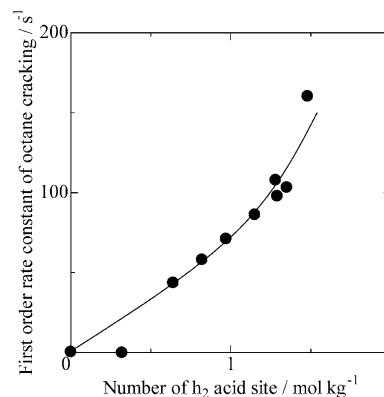


Naonobu Katada, Yasuyoshi Kageyama, Kazue Takahara, Takahide Kanai, Hosne Ara Begum, Miki Niwa

Journal of Molecular Catalysis A: Chemical 211 (2004) 119

Acidic property of modified ultra stable Y zeolite: increase in catalytic activity for alkane cracking by treatment with ethylenediaminetetraacetic acid salt

Strong Brønsted acid sites were increased by the treatment of an ultra stable Y (USY) zeolite with a sodium salt of ethylenediaminetetraacetic acid, as indicated by temperature-programmed desorption of ammonia. The catalytic activity for alkane cracking was also enhanced, suggesting that the active site of USY for the catalytic cracking is this strong Brønsted acid site.

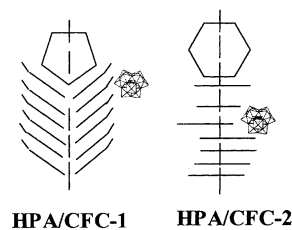


M.N. Timofeeva, M.M. Matrosova, T.V. Reshetenko, L.B. Avdeeva, A.A. Budneva, A.B. Ayupov, E.A. Paukshtis, A.L. Chuvilin, A.V. Volodin, V.A. Likhonolobov

Journal of Molecular Catalysis A: Chemical 211 (2004) 131

Filamentous carbons as a support for heteropoly acid

The different kinds of catalytic filamentous carbons were used as a support for heteropoly acids: H₆P₂W₂₁O₇₁ (H₂O)₃, H₆As₂W₂₁O₆₉ (H₂O), α-H₆P₂W₁₈O₆₂ (P₂W₁₈) and H₃PW₁₂O₄₀ (PW). Concentration of Brønsted acidic sites of supported and bulk PW was determined from ESR studies of the stable nitroxyl radical. The reaction of 2,6-di-*tert*-butyl-4-methylphenol with toluene was studied using bulk and supported PW and P₂W₁₈.

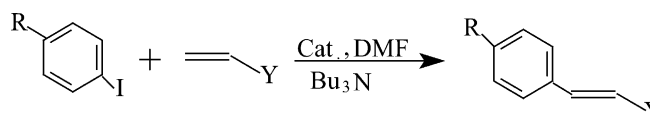


Shao Fen Zhao, Ren Xian Zhou, Xiao Ming Zheng

Journal of Molecular Catalysis A: Chemical 211 (2004) 139

Heterogeneous Heck reaction catalyzed by a series of amine–palladium(0) complexes

A series of polymeric amine–palladium(0) complexes have been prepared from organic silica via immobilization on fumed silica. They are efficient catalysts for Heck arylation of aryl iodides with alkene and can be recovered and reused.

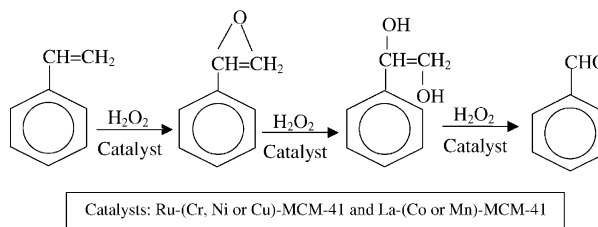


V. Pârvulescu, C. Anastasescu, B.L. Su

Journal of Molecular Catalysis A: Chemical 211 (2004) 143

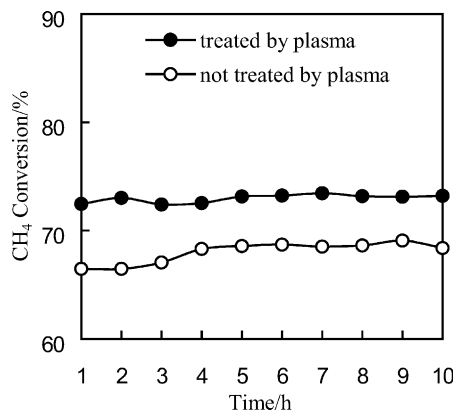
Bimetallic Ru-(Cr, Ni, or Cu) and La-(Co or Mn) incorporated MCM-41 molecular sieves as catalysts for oxidation of aromatic hydrocarbons

The catalytic activity of bimetallic Ru-(Co, Ni, Cu) and La-(Co or Mn) modified-MCM-41 molecular sieves in liquid phase selective oxidation with hydrogen peroxide shows a very high conversion in hydroxylation of benzene to phenol, but a lower activity in oxidation of styrene to benzaldehyde, being contrary to that of monometallic modified MCM-41 catalysts.


Zhen-Hua Li, Shu-Xun Tian, Hai-Tao Wang, Hong-Bing Tian

Journal of Molecular Catalysis A: Chemical 211 (2004) 149

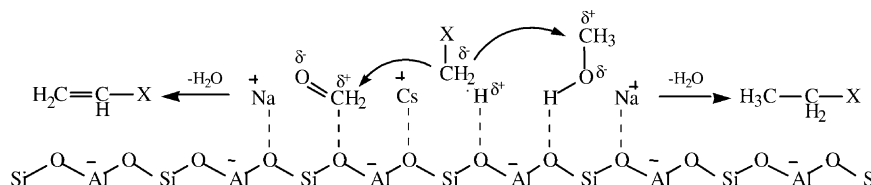
Plasma treatment of Ni catalyst via a corona discharge


Tawan Sooknoi, John Dwyer

Journal of Molecular Catalysis A: Chemical 211 (2004) 155

Role of substrate's electrophilicity in base catalysis by zeolites: alkylation of acetonitrile with methanol

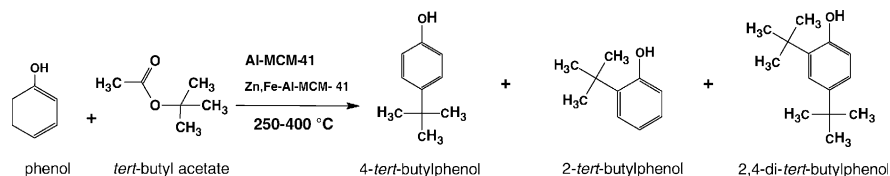
“On the high polar surface of CsNaX, an electrophilic substrate (CH_3X) is adsorbed and a carbanion-like intermediate is formed on the caesium countered site. Such species can either react with methanol or formaldehyde adsorbed on the sodium countered sites forming saturated and unsaturated alkylate products, respectively”.


R. Savidha, A. Pandurangan, M. Palanichamy, V. Murugesan

Journal of Molecular Catalysis A: Chemical 211 (2004) 165

A comparative study on the catalytic activity of Zn and Fe containing Al-MCM-41 molecular sieves on *t*-butylation of phenol

Incorporation of Zn and Fe in Al-MCM-41 framework is found to increase the total acidity of catalysts and the incorporated Fe(III) is found to be in tetrahedral co-ordination. *t*-Butylation of phenol with a new alkylating agent, *t*-butyl acetate was carried over Al-MCM-41, Zn- and Fe-Al-MCM-41 in vapour phase and found that the phenol conversion and 4-*t*-butyl phenol selectivity are higher over Zn- and Fe-Al-MCM-41 than that of Al-MCM-41 catalysts.

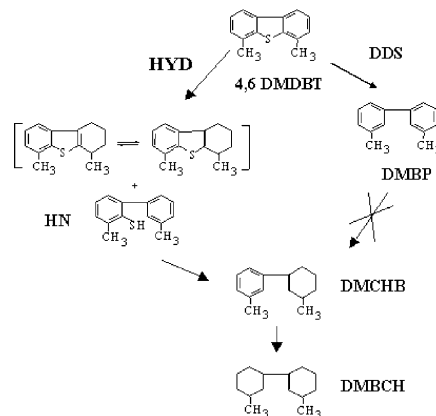


D. Zuo, D. Li, H. Nie, Y. Shi, M. Lacroix, M. Vrinat

Journal of Molecular Catalysis A: Chemical 211 (2004) 179

Acid–base properties of NiW/Al₂O₃ sulfided catalysts: relationship with hydrogenation, isomerization and hydrodesulfurization reactions

Effect of the promoter over the acid–base and catalytic properties of sulfided catalysts was investigated by comparison of a series of NiW/Al₂O₃ (with constant tungsten loading and variable nickel content) in HDS of 4,6-DMDBT (4,6-dimethyldibenzothiophene), and isomerization of *o*-xylene. Association of both reactions was found to be very useful to prove the effect of Ni on hydrogen activation (Bronsted acid site formation) and on the elimination process (basicity of S²⁻ centers).



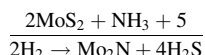
Y.J. Lee, T.H. Nguyen, A. Khodakov, A.A. Adesina

Journal of Molecular Catalysis A: Chemical 211 (2004) 191

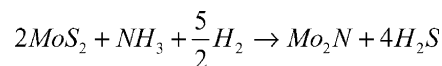
Physicochemical attributes of oxide supported Mo₂N catalysts synthesised via sulphide nitridation

This study deals with a new route for the preparation of high surface area Mo₂N from supported MoS₂ synthesised via precipitation from homogeneous solution.

The Mo sulphide nitridation reaction is given by:



Alumina supported Mo₂N gave the best surface area and CO hydrogenation activity (when used as a catalyst).

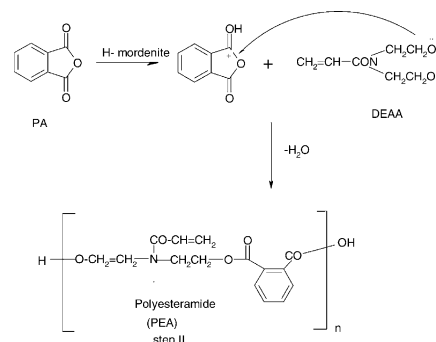


Mohamed Mokhtar Mohamed, F. Abd El-Hai

Journal of Molecular Catalysis A: Chemical 211 (2004) 199

Catalytic polymerization of *N,N*-diethanol acrylamide with phthalic anhydride in the presence of H-mordenite and Fe-mordenite zeolites

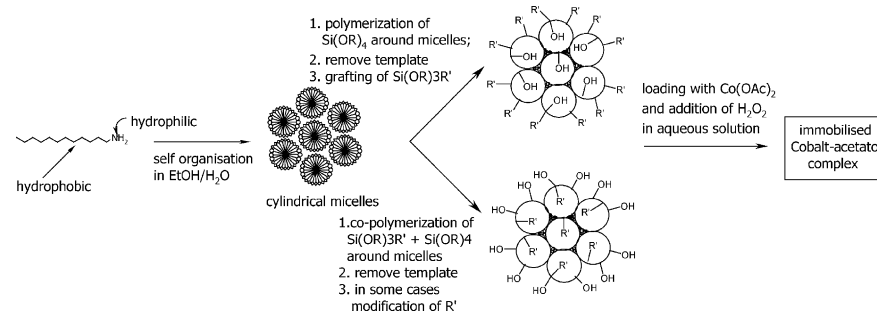
H-mordenite zeolite was shown to be a recyclable catalyst for *N,N*-diethanol acrylamide (DEAA; 91% selectivity) with phthalic anhydride (PA) yielding polyesteramide (PEA, 100% selectivity) resin in only 30 min.



Timo Pruß, Duncan J. Macquarrie, James H. Clark

Journal of Molecular Catalysis A: Chemical 211 (2004) 209

Cobalt–acetato complexes immobilised on PYP A-organomodified silica: a case study of different ways of immobilisation

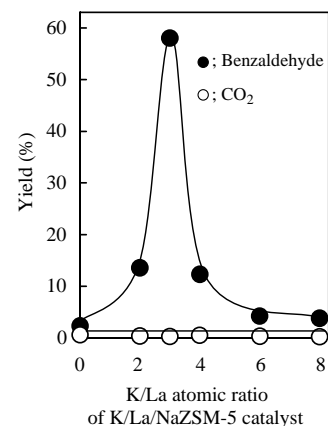


**Masaya Furukawa, Yoko Nishikawa,
Satoru Nishiyama, Shigeru Tsuruya**

Journal of Molecular Catalysis A: Chemical 211 (2004) 219

Effect of alkali metal added to supported La catalysts on the catalytic activity in the gas-phase catalytic oxidation of benzyl alcohol

The addition of alkali metal to the lanthanum catalysts supported on NaZSM-5 and SiO₂ selectively promoted the partial oxidation in the gas-phase catalytic oxidation of benzyl alcohol.

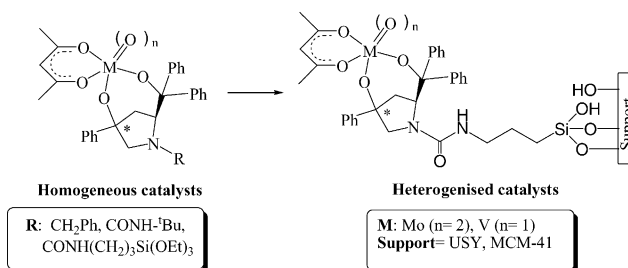


A. Fuerte, M. Iglesias, F. Sánchez, A. Corma

Journal of Molecular Catalysis A: Chemical 211 (2004) 227

Chiral dioxomolybdenum(VI) and oxovanadium(V) complexes anchored on modified USY-zeolite and mesoporous MCM-41 as solid selective catalysts for oxidation of sulfides to sulfoxides or sulfones

Several chiral dioxomolybdenum and oxovanadium complexes, homogeneous and heterogenised on modified USY-zeolite and mesoporous MCM-41, have been investigated as catalysts in the selective oxidation of sulfides to sulfoxides or sulfones; the new catalysts are highly suited to reactions leading to high yields and excellent selectivity to sulfoxide formation. The possibility of recycling of molybdenum heterogenised catalysts is demonstrated.

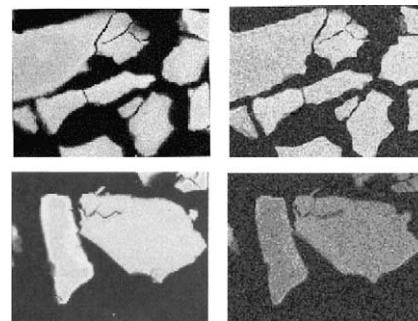


**B. Corain, P. Guerriero, G. Schiavon,
M. Zapparoli, M. Kralik**

Journal of Molecular Catalysis A: Chemical 211 (2004) 237

Generation of a silica skeleton inside of gel-type functional resins supporting catalytically active palladium nanoclusters

The pictures show silicon (left) and palladium (right) distribution (XRMA) through the section of the particles (180–400 μm) of the as prepared hybrid organic–inorganic nanocomposite β-MPIF⁻Na⁺/Pd⁰/SiO₂ (upper figure) and of the same material after thermal treatment up to 600 °C under nitrogen (lower figure). The severe treatment does not alter silicon and palladium distribution.



**Yan Pei, Huarong Hu, Jing Fang,
Minghua Qiao, Weilin Dai, Kangnian Fan,
Hexing Li**

Journal of Molecular Catalysis A: Chemical 211 (2004) 243

Liquid phase hydrogenation of crotonaldehyde over Sn-promoted amorphous Co–B catalysts

Four kinds of tin (Sn)-promoted amorphous Co–B catalysts have been investigated in the liquid phase hydrogenation of crotonaldehyde. The 1% SnCl₄ Co–B catalyst showed a high selectivity to crotyl alcohol by depressing the reactivity of the C=C bond while increasing the reactivity of the C=O bond.

