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## R. Mary Magdalene, E.G. Leelamani, N.M. Nanje Gowda

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Hydrogenation of nitroarenes using polybenzimidazole-supported rhodium catalyst

## R. Ganesan, B. Viswanathan

Journal of Molecular Catalysis A: Chemical 223 (2004) 21

Redox properties of bis(8-hydroxyquinoline)manganese(II) encapsulated in various zeolites

Bis(8-hydroxyquinoline)manganese(II) [Mn (C<sub>9</sub>H<sub>6</sub>NO)<sub>2</sub>] (Mn-Qn) was encapsulated in NaY, KL, MCM-41, Naβ and NaZSM-5. Characterization of the catalyst was done by using IR, UV-vis and EPR spectroscopy. The redox properties of neat and encapsulated Mn-Qn complexes were studied by cyclic voltammetry. The redox potential of metal complex was altered when Mn-Qn complex was encapsulated in various zeolites. Similar trend was observed when cytochrome-C was immobilized on MCM-41. The change in the position of HOMO and LUMO level of Mn-Qn complexes upon encapsulation in various zeolites were calculated by using density functional theory. The catalytic activity towards oxidation of cyclohexanol was performed using neat and encapsulated Mn-Qn complexes. The Mn-Qn complex encapsulated in NaY and KL zeolites is only showing higher activity for the oxidation of cyclohexanol.

## Vaibhav B. Valodkar, Gopal L. Tembe, Marayil Ravindranathan, H.S. Rama

Journal of Molecular Catalysis A: Chemical 223 (2004) 31

Catalytic oxidation of alkanes and alkenes by polymer-anchored amino acid-ruthenium complexes

#### Rajesh Chakrabarty, Birinchi K. Das

Journal of Molecular Catalysis A: Chemical 223 (2004) 39

Epoxidation of  $\alpha$ -pinene catalysed by tetrameric cobalt(III) complexes

A tetrameric cobalt(III) complex  $[Co_4(\mu_3-O)_4(\mu-C_6H_5CO_2)_4(4-CNpy)_4]$  (I) containing a  $[Co^{III}_4(\mu_3-O)_4]$  cubane core catalyses the homogeneous air oxidation of  $\alpha$ -pinene under atmospheric pressure. High selectivity (62–68%) for  $\alpha$ -pinene oxide formation is observed.

## Nandkumar M. Patil, Ashutosh A. Kelkar, Raghunath V. Chaudhari

Journal of Molecular Catalysis A: Chemical 223 (2004) 45

Synthesis of triarylamines by copper-catalyzed amination of aryl halides

A simple and efficient methodology for the synthesis of triphenylamine (TPA) in a single step has been demonstrated using copper catalyst with a ligand. The effect of parameters such as catalyst precursors, ligands, bases and solvents on the activity and selectivity to triphenylamine were investigated and best result was obtained using 2,6-diphenylpyridine as a ligand (94% yield of TPA).

## Ganapati D. Yadav, Piyush S. Lathi

Journal of Molecular Catalysis A: Chemical 223 (2004) 51

Synergism between microwave and enzyme catalysis in intensification of reactions and selectivities: transesterification of methyl acetoacetate with alcohols

The rates of transesterification of methyl acetoacetate with a variety of alcohols such as n-propanol, n-butanol, n-pentanol, n-hexanol, n-octanol and n-decanol by using Novozym 435 were enhanced by a factor of 2.2–4.6 in the presence of microwave irradiation.

$$H_{3}C$$
 $OCH_{3}$ 
 $+$  ROH
 $OCH_{3}$ 
 $+$  ROH
 $OCH_{3}$ 
 $+$  CH<sub>3</sub>OH

# Bhanu M. Chanda, Renu Vyas, Sudhir S. Landge

Journal of Molecular Catalysis A: Chemical 223 (2004) 57

Synthesis of aziridines using new catalytic systems with bromamine-T as the nitrene source

#### Manish K. Mishra, Beena Tyagi, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 223 (2004) 61

Synthesis and characterization of nano-crystalline sulfated zirconia by sol-gel method

Synthesis of nano-crystalline sulfated zirconia with crystallite size of 20 nm using the one-step as well as two-step sol-gel technique. In the one-step method, sample prepared by adding sulphuric acid in zirconium alkoxide precursor before the addition of water showed improved structural and textural properties.

#### Hillary A. Prescott, Martin Wloka, Erhard Kemnitz

Journal of Molecular Catalysis A: Chemical 223 (2004) 67

Supported sulfated zirconia catalysts and their properties

Sulfated zirconia (SZ),  $SO_4/ZrO_2$ , was supported by  $SiO_2$ ,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, and K-10. Aspects of preparation, such as  $ZrO_2$  precursor, sulfur contents, sulfating agent, and calcination conditions, were varied. The pure supports and catalysts were characterized with XRD, BET, FTIR photoacoustic spectroscopy (pyridine adsorption), NH<sub>3</sub>-TPD, and tested for the benzoylation of anisole with benzoyl chloride. The support strongly affects the catalytic activity.

## M.V. Alexander, A.C. Khandekar, S.D. Samant

Journal of Molecular Catalysis A: Chemical 223 (2004) 75

Sulfonylation reactions of aromatics using FeCl<sub>3</sub>-based ionic liquids

$$\begin{array}{c|c} R & & SO_2CI \\ \hline & & \\ \hline & &$$

and [bmim]Cl =  $\prod_{N}$ 

# Anand B. Shivarkar, Sunil P. Gupte, Raghunath V. Chaudhari

Journal of Molecular Catalysis A: Chemical 223 (2004) 85

Carbamate synthesis via transfunctionalization of substituted ureas and carbonates

Synthesis of carbamates from substituted ureas and organic carbonates has been demonstrated using n-dibutyl tin oxide (DBTO) as a catalyst. In a typical case 91% yield of N-methyl methyl carbamate have been obtained.

NHR<sup>1</sup> 
$$OR^2$$

$$+ OR^2$$

$$+ OR^2$$

$$NHR^1 OR^2$$

$$+ OR^2$$

$$+$$

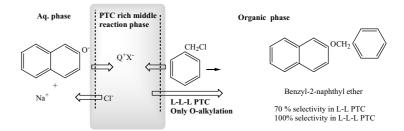
 $R^{1}, R^{2}$  = aliphatic or aromatic

#### Ganapati D. Yadav, Priyal M. Bisht

Journal of Molecular Catalysis A: Chemical 223 (2004) 93

Selectivity engineering in multiphase transfer catalysis in the preparation of aromatic ethers

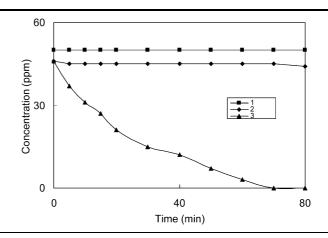
A 100% selectivity of the ether is obtained by using L–L–L PTC process as against the 70% using L–L PTC and the reaction occurs in the middle catalyst rich phase in the triphasic system.



# S. Lathasree, A. Nageswara Rao, B SivaSankar, V. Sadasivam, K. Rengaraj

Journal of Molecular Catalysis A: Chemical 223 (2004) 101

Heterogeneous photocatalytic mineralisation of phenols in aqueous solutions



## Amrita S. Kulkarni, Radha V. Jayaram

Journal of Molecular Catalysis A: Chemical 223 (2004) 107

Liquid phase catalytic transfer hydrogenation of aromatic nitro compounds on  $La_{1-x}Sr_xFeO_3$  perovskites prepared by microwave irradiation

A series of perovskites of the type  $\text{La}_{1-x}\text{Sr}_x\text{FeO}_3$  (x=0.0-1.0) prepared by conventional and microwave irradiation method were used to study the liquid phase catalytic transfer hydrogenation of aromatic nitro compounds.

#### Devendrapratap U. Singh, Shriniwas D. Samant

Journal of Molecular Catalysis A: Chemical 223 (2004) 111

Comparative study of benzylation of benzene using benzyl chloride in the presence of pillared bentonite; ion-exchanged and pillaring solution impregnated montmorillonite K10

$$R = -H, -CH_3, -C_2H_5, -CH(CH_3)_2, -OCH_3, -Cl, -Br$$

## C. Ravindra Reddy, B. Vijayakumar, Pushpa Iyengar, G. Nagendrappa, B.S. Jai Prakash

Journal of Molecular Catalysis A: Chemical 223 (2004) 117

Synthesis of phenylacetates using aluminium-exchanged montmorillonite clay catalyst

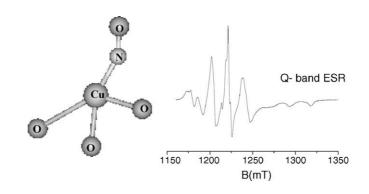
Liquid phase esterification of phenylacetic acid with phenol and substituted phenols has been investigated over montmorillonite clay exchanged with H<sup>+</sup>-, Al<sup>3+</sup>- and aluminium polyhydroxy oligomer cations. Among the catalysts studied, Al<sup>3+</sup>—montmorillonite dried at 100 °C showed 67% conversion, while the same catalyst dried at 200 °C showed reduced conversion of 36%. Al<sup>3+</sup>—montmorillonite dried at 400 °C and montmorillonite exchanged with aluminium polyhydroxy oligomer cations dried at 100 °C and calcined at 500 °C failed to bring about the reaction. Effects of mole ratio of reactants, reaction period and catalyst amount on yield of the ester and catalyst regeneration are also investigated.

CH<sub>2</sub>COOH + R 
$$\rightarrow$$
 OH  $\rightarrow$  Catalyst  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  P  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  P  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  P  $\rightarrow$  CH<sub>2</sub>COO  $\rightarrow$  CH<sub>2</sub>COO

#### V. Umamaheswari, Andreas Pöppl, Martin Hartmann

Journal of Molecular Catalysis A: Chemical 223 (2004) 123

Electron spin resonance spectroscopy of Cu(I)–NO complexes in copper exchanged zeolites



# H. Kathyayini, N. Nagaraju, A. Fonseca, J.B. Nagy

Journal of Molecular Catalysis A: Chemical 223 (2004) 129

Catalytic activity of Fe, Co and Fe/Co supported on Ca and Mg oxides, hydroxides and carbonates in the synthesis of carbon nanotubes

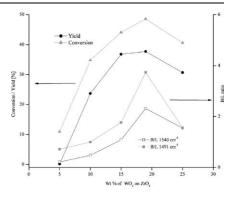
Multiwall carbon nanotubes are produced by CCVD of acetylene/ethlyne at 700 °C in the presence of different Mg and Ca salts supported Fe, Co and Fe/Co catalyst systems. MgO/Fe–Co gave the best yield (238%). The nanotubes could be purified using HCl.

## R. Sakthivel, H. Prescott, E. Kemnitz

Journal of Molecular Catalysis A: Chemical 223 (2004) 137

WO<sub>3</sub>/ZrO<sub>2</sub>: a potential catalyst for the acetylation of anisole

WO<sub>3</sub>/ZrO<sub>2</sub> catalysts (5–25wt.% WO<sub>3</sub>) were prepared by coprecipitation and characterized with XRD, BET, FTIR (pyridine adsorption), and NH<sub>3</sub>-TPD. Their activities were tested in the acetylation of anisole with acetic anhydride. The relationship between the catalytic activities found and the Brønsted/Lewis acid site ratio dependent on the WO<sub>3</sub> loadings was examined and is discussed.



# S. Shanmugam, B. Viswanathan, T.K. Varadarajan

Journal of Molecular Catalysis A: Chemical 223 (2004) 143

Esterification by solid acid catalysts—a comparison

The esterification of triethylene glycol (TEG) with methacrylic acid (MAA) was carried out over various solid acid catalysts and the results are compared with that of conventional acid catalysts. Among the catalysts studied, heteropolyacids showed higher activities than the conventional acids. Parameters such as activation energy, reaction enthalpy and reaction entropy were derived for this reaction over phosphotungstic acid in the temperature range of 353–383 K.

HO
$$^{O}$$
O $^{O}$ OH + 2 OH  $^{O}$ OH  $^{O$ 

Triethylene glycol

Methacrylic acid

Triethyelene glycol dimethacrylate

# Ch. Subrahmanyam, B. Viswanathan, T.K. Varadarajan

Journal of Molecular Catalysis A: Chemical 223 (2004) 149

Synthesis, characterization and catalytic activity of mesoporous trivalent iron substituted aluminophosphates Trivalent iron incorporated mesoporous aluminophosphate was synthesized and characterized. Activity of Fe-AlPO was tested for aerial oxidation of cyclohexane under autoclave conditions. The results indicated that Fe-AlPO is an active catalyst for oxidation of cyclohexane and the reaction is probably taking place through radical initiated mechanism.

#### G. Kuriakose, N. Nagaraju

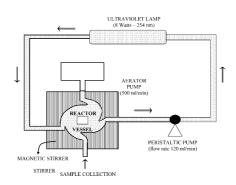
Journal of Molecular Catalysis A: Chemical 223 (2004) 155

Selective synthesis of phenyl salicylate (salol) by esterification reaction over solid acid catalysts

## B. Swarnalatha, Y. Anjaneyulu

Journal of Molecular Catalysis A: Chemical 223 (2004) 161

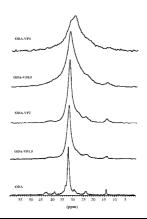
Studies on the heterogeneous photocatalytic oxidation of 2,6-dinitrophenol in aqueous  ${\rm TiO}_2$  suspension



#### Soumen Dasgupta, Monika Agarwal, Arunabha Datta

Journal of Molecular Catalysis A: Chemical 223 (2004) 167

Mesolamellar vanadium phosphate phases obtained by intercalation of a long chain alkylamine into different catalytically important VPO host lattices



#### K. Shanmugapriya, S. Saravanamurugan, M. Palanichamy, Banumathi Arabindoo, V. Murugesan

Journal of Molecular Catalysis A: Chemical 223 (2004) 177

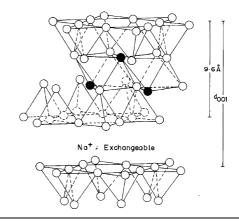
Alkylation and acylation of phenol with methyl acetate

The vapour phase reaction of phenol with methyl acetate was investigated over MgZSM-5, MgY and Mg $\beta$  zeolites. The activity of the catalysts at 400 °C followed the order Mg $\beta$  > MgZSM-5  $\approx$  MgY which was also the order of Lewis acidity. 4-Methyl coumarin was observed over Mg $\beta$  at a feed ratio of 1:5.

#### Thiripuranthagan Sivakumar, Thangavelu Krithiga, Kannan Shanthi, Tohru Mori, Jun Kubo, Yutaka Morikawa

Journal of Molecular Catalysis A: Chemical 223 (2004) 185

Noble metals intercalated/supported mica catalyst – synthesis and characterization

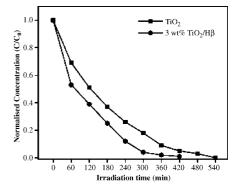


#### M.V. Shankar, K.K. Cheralathan, Banumathi Arabindoo, M. Palanichamy, V. Murugesan

Journal of Molecular Catalysis A: Chemical 223 (2004) 195

Enhanced photocatalytic activity for the destruction of monocrotophos pesticide by  $\text{TiO}_2/\text{H}\beta$ 

Supporting  $TiO_2$  on  $H\beta$  zeolite improves its photocatalytic activity for the destruction of aqueous monocrotophos (MCP) pesticide, a known endocrine disruptor. This improved activity is due to the greater adsorption of MCP by the zeolite support and its capability to delocalise the conduction band electrons of excited  $TiO_2$ .



#### K. Usha Nandhini, Banumathi Arabindoo, M. Palanichamy, V. Murugesan

Journal of Molecular Catalysis A: Chemical 223 (2004) 201

*t*-Butylation of phenol over mesoporous aluminophosphate and heteropolyacid supported aluminophosphate molecular sieves Mesoporous aluminophosphate supported phosphotungstic acid (10, 20 and 40 wt.% PW/AlPOs) catalysts were synthesized and characterized for vapour phase alkylation of phenol with *t*-butanol. The products were *o-tert*-butyl phenol (*o-t*-BP), *p-tert*-butyl phenol (*p-t*-BP) and *tert*-butyl phenyl ether (*t*-BPE). These catalysts were found to be more active than parent AlPO due to increase in Bronsted acid sites. The order of the activity of the catalysts was found to be 20 wt.% PW/AlPO > 40 wt.% PW/AlPO > 10 wt.% PW/AlPO.

#### Shyam Kishore Roy, P. Dutta, L.N. Nandi, S.N. Yadav, T.K. Mondal, S.C. Ray, Swapan Mitra, P. Samuel

Journal of Molecular Catalysis A: Chemical 223 (2004) 211

The influence of support on ammoxidation of 3-picoline over vanadia catalyst

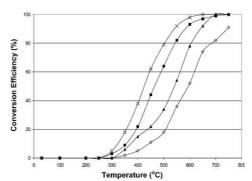
The influence of high content of  $MoO_3$  (32 mol%) in  $V_2O_5$ - $MoO_3$ - $P_2O_5$  catalyst system supported on alumina, silica, HZSM-5 and modified clay was investigated for ammoxidation of 3-picoline. Major intermediate phases identified are  $Mo_4V_6O_{25}$ ,  $Mo_6V_9O_{40}$ ,  $MoV_2O_8$ . FT-IR spectra and X-ray diffractograms showed interaction among the active oxides and the support. The physico-chemical properties of the catalysts were correlated with their activity and selectivity for ammoxidation of 3-picoline.

## Nitin K. Labhsetwar, A. Watanabe, T. Mitsuhashi, H. Haneda

Journal of Molecular Catalysis A: Chemical 223 (2004) 217

Thermally stable ruthenium-based catalyst for methane combustion

 $La_{3.5}Ru_{4.0}O_{13} \ type \ ruthenium (IV) \ based \ perovskite \ has been \ synthesized \ in \ supported \ and \ unsupported \ forms. \ They show high thermal stability and good catalytic activity for methane combustion reaction.$ 



## D. Kishore, S. Kannan

Journal of Molecular Catalysis A: Chemical 223 (2004) 225

Environmentally benign route for isomerization of safrole—hydrotalcite as solid base catalyst

Isomerization of safrole to isosafrole, an important double bond migration reaction, is carried out over MgM(III) hydrotalcites, where M(III) = Al, Fe and Cr. Among the catalysts studied, MgAl hydrotalcite with Mg/Al atomic ratio 6.0 showed maximum conversion of around 98% with a *cisltrans* isosafrole ratio of 1/9 at 200  $^{\circ}$ C using DMSO as solvent. Bronsted basic hydroxyl groups attached to Mg<sup>2+</sup> are proposed as the active centers involved in the isomerization reaction.

## P. Dutta, S.C. Roy, L.N. Nandi, P. Samuel, S. Muthukumaru Pillai, B.D. Bhat, M. Ravindranathan

Journal of Molecular Catalysis A: Chemical 223 (2004) 231

Synthesis of lower olefins from methanol and subsequent conversion of ethylene to higher olefins via oligomerisation Tungstophosphoric acid and Cesium salt exhibit activity for conversion of methanol to lower olefins like ethylene and propylene. In liquid phase  $TiCl_4$  and  $Ti(OBu)_4$  based systems are good oligomerization catalysts of ethylene to give  $C_4$ – $C_{14}$  alpha olefins. On the otherhand in vapour phase HZSM-5, Ni-SAPO-5 produce  $C_4$ – $C_6$  saturates and olefins from ethylene.

HPW = Tungstophosphoric acid

n 
$$\operatorname{CH_2=CH_2} \xrightarrow{\operatorname{Catalyst}} \operatorname{C}_2\operatorname{H}_5\text{-}\operatorname{CH=CH}_2, \operatorname{C}_4\operatorname{H}_9\operatorname{CH=CH}_2$$
 etc

Catalyst = Ti R<sub>4</sub> - Et<sub>3</sub>Al<sub>2</sub>Cl<sub>3</sub> where R = Cl, OBu

 $\label{eq:CH2CH2CH3} \mbox{Catalyst} \\ \mbox{n $\operatorname{CH}_2$=$\operatorname{CH}_2$$} \longrightarrow \mbox{CH}_3 \mbox{CH}_2 \mbox{CH}_2 \mbox{CH}_3, \mbox{CH}_2 \mb$ 

Catalyst = HZSM-5, Ni-SAPO-5 etc

### Rutuja D. Tilve, M. Varughese Alexander, Amit C. Khandekar, Sriniwas D. Samant, Vinod R. Kanetkar

Journal of Molecular Catalysis A: Chemical 223 (2004) 237

Synthesis of 2,3-unsaturated glycopyranosides by Ferrier rearrangement in FeCl<sub>3</sub> based ionic liquid

where R = alkyl.

## S.E. Dapurkar, A. Sakthivel, P. Selvam

Journal of Molecular Catalysis A: Chemical 223 (2004) 241

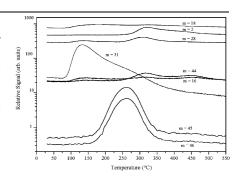
Mesoporous VMCM-41: highly efficient and remarkable catalyst for selective oxidation of cyclohexane to cyclohexanol

Mesoporous VMCM-41 is a very efficient and highly selective for the oxidation of cyclohexane to cyclohedanol under mild conditions, and that it also shows excellent recycling ability thus behaves truly as heterogeneous catalyst.

# Dharmesh Kumar, S. Varma, V.S. Kamble, N.M. Gupta

Journal of Molecular Catalysis A: Chemical 223 (2004) 251

The selective adsorption/reaction of methanol over nanosize uranium oxide crystallites dispersed in MCM-48: FT-IR and TPD studies In situ FTIR and TPD-MS studies reveal that the transient species formed during adsorption of methanol were different on  $U_3O_8$  crystallites dispersed over mesoporous MCM-48, as compared to those over bulk  $U_3O_8$  or host matrix alone. While the formate complexes were the main intermediates over bulk  $U_3O_8$ , methoxide, oxymethylene and polymerized oxymethylene species were formed over dispersed samples that helped in the selective oxidation of methanol to form formaldehyde and formic acid in addition to the oxides of carbon.



#### S.A.R. Mulla, V.R. Choudhary

Journal of Molecular Catalysis A: Chemical 223 (2004) 259

Oxidative conversion of ethane to ethylene over supported SrO-promoted Er<sub>2</sub>O<sub>3</sub> catalyst

Oxidative conversion of ethane to ethylene over a SrO-promoted  ${\rm Er_2O_3}$  supported on low surface area macroporous silica-alumina commercial catalyst carrier in presence of steam and limited  ${\rm O_2}$  at different temperature,  ${\rm C_2H_6/O_2}$  feed ratio and space velocity has been thoroughly investegated.

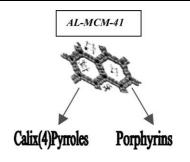
$$C_2H_6 \quad + \quad O_2 \quad \rightarrow \quad C_2H_4 \quad + \quad H_2O$$

#### M. Radha Kishan, V. Radha Rani, M.R.V.S. Murty, P. Sita Devi, S.J. Kulkarni, K.V. Raghavan

Journal of Molecular Catalysis A: Chemical 223 (2004) 263

Synthesis of calixpyrroles and porphyrins over molecular sieve catalysts

The selective liquid phase synthesis of calix (4) pyrroles and porphyrins was accomplished using different zeolite catalysts, under microwave conditions. Mesoporous Al-MCM-41 offered quantitative conversions when compared to other catalysts as monitored by HPTLC.

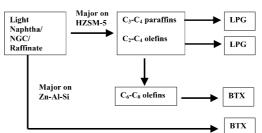


## N. Viswanadham, G. Muralidhar, T.S.R. Prasada Rao

Journal of Molecular Catalysis A: Chemical 223 (2004) 269

Cracking and aromatization properties of some metal modified ZSM-5 catalysts for light alkane conversions

Cracking and aromatisation of various hydrocarbon components present in industrial feedstocks such as Natural Gas Condensate (NGC), light naphtha and raffinate on H-ZSM-5, Zn and Ga incorporated ZSM-5 were studied. A Zn-Al-Si catalyst prepared by framework incorporation of Zn exhibited low acidity and cracking activity that produced 50–65wt.% aromatics along with 21–33wt.% of LPG as a by-product which has significant impact on Indian industry, where high octane gasoline and LPG are in great demand.

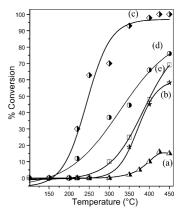


# Mrinal R. Pai, B.N. Wani, A.D. Belapurkar, N.M. Gupta

Journal of Molecular Catalysis A: Chemical 223 (2004) 275

Role of substitution in catalytic activity of La-Th-V-O mixed oxides for the reaction of methanol

La doping to the extent of 20% resulted in the improved catalytic activity of  $ThV_2O_7$  for the dehydrative conversion of methanol to form dimethyl ether, methane and carbon dioxide. In addition, the substituted samples exhibited better stoichiometric stability during the repeated cycles of reduction/oxidation. The role of secondary phases generated due to substitution is discussed.



V. Siva Kumar, B.M. Nagaraja, V. Shashikala, P. Seetharamulu, A.H. Padmasri,

B. David Raju, K.S. Rama Rao

Journal of Molecular Catalysis A: Chemical 223 (2004) 283

Role of acidic and basic sites of  $Al_2O_3$  in predicting the reaction pathway of isophorone transformation

In the armatization of isophorone, acidic and basic sites play a crucial role. Masking of either acidic or basic sites of aluminum oxide, by co-feeding of NH<sub>3</sub> or CO<sub>2</sub>, respectively, along with isophorone, indicate the involvement of weak/moderate basic sites to abstract a proton to form an enolate ion followed by involvement of weak/moderate acid sites for dienone–phenol rearrangement to yield aromatization products and involvement of strong acidic sites for yielding decomposition products.

$$H_3C$$
 $H_3C$ 
 $CH_3$ 
 $H_3C$ 
 $CH_3$ 
 $H_3C$ 
 $CH_3$ 
 $AI_2O_3$ , WHSV = 1.0 h<sup>-1</sup>
 $CH_4$ 
 $CH_4$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 

### Rajesh Gopinath, N. Lingaiah, N. Seshu Babu, I. Suryanarayana, P.S. Sai Prasad, Akira Obuchi

Journal of Molecular Catalysis A: Chemical 223 (2004) 289

A highly active low Pd content catalyst synthesized by deposition–precipitation method for hydrodechlorination of chlorobenzene

Hydrodechlorination of chlorobenzene was studied over 1 wt.% Pd supported on  $ZrO_2$  synthesized by deposition-precipitation and conventional impregnation methods using chloride and nitrate salts of Pd. The catalysts were characterized by CO chemisorption, BET surface area, XPS and temperature-programmed reduction. The catalyst prepared by the DP method using chloride precursor has shown the highest activity and stability compared to the other catalysts. This is a significant observation in terms of considerable reduction in palladium content. The variation in chlorobenzene conversion of different catalysts is explained based on the nature of Pd species formed on the surface.

CI + 
$$H_2$$
  $\frac{1 \text{wt\%Pd/ZrO}_2}{140\text{-}200\,^{\circ}\text{C}}$  +  $HCI$ 

#### Benjaram M. Reddy, Ibram Ganesh, Ataullah Khan

Journal of Molecular Catalysis A: Chemical 223 (2004) 295

Stabilization of nanosized titania-anatase for high temperature catalytic applications

 $M_2O_3$ -TiO<sub>2</sub> and  $V_2O_5/M_2O_3$ -TiO<sub>2</sub> (M = Ga, In and La) nanosized mixed oxide catalysts were investigated by various techniques to understand surface structure, dispersion and temperature stability. These catalysts were also evaluated for one step synthesis of 2,6-dimethylphenol from cyclohexanone and methanol in the vapour phase.

# C.P. Sebastian, Shivanand Pai, N. Sharanappa, C.V.V. Satyanarayana

Journal of Molecular Catalysis A: Chemical 223 (2004) 305

Regio selective butylation of toluene on mordenite catalysts: influence of acidity

During alkylation of toluene with tert-butyl alcohol in the presence of mordenite catalyst the primary product expected to be formed is p-tert-butyltoluene as a result of o/p directing effect of alkyl group and also o-tert-butyltoluene is not formed inside zeolite pores due to its bulky nature. The m-tert-butyltoluene is formed through acid catalysed isomerisation of p-tert-butyltoluene, mostly on the external surface. By appropriate choice of  $SiO_2/Al_2O_3$  ratio and operating conditions the selectivity to p-tert-butyltoluene can be maximized.

V. Siva Kumar, B.M. Nagaraja, V. Shashikala, A.H. Padmasri, S. Shakuntala Madhavendra, B. David Raju, K.S. Rama Rao

Journal of Molecular Catalysis A: Chemical 223 (2004) 313

Highly efficient Ag/C catalyst prepared by electrochemical deposition method in controlling microorganisms in water The silver nano-particles prepared by electro-chemical method deposited on activated carbon (AgC-EC) are found to be highly efficient in controlling microorganisms in water. The advantages of this catalyst over the silver catalysts obtained by conventional impregnation technique are demonstrated in this report. This method yields silver nano-particles directly in metallic form unlike the conventional technique. Thus for the catalyst AgC-EC, no pretreatment is needed for controlling the microorganisms in water. Hence, it is more cost effective as the pretreatment processes viz., calcinations and/or reduction can be avoided with the electro-chemical deposition method. Whereas the silver catalysts prepared by conventional impregnation technique require reduction prior to use in controlling microorganisms in water because silver is in oxidic form.

- R-S-H + O + H - S - R- 
$$\longrightarrow$$
 - R - S - S - R- + H<sub>2</sub>O Destruction of cell membrane surface of microorganisms by silver nano-particles

K.V. Narayana, B. David Raju, S. Khaja Masthan, V. Venkat Rao, P. Kanta Rao, A. Martin

Journal of Molecular Catalysis A: Chemical 223 (2004) 321

Cerium fluoride supported  $V_2O_5$  catalysts: physico-chemical characterization and 3-picoline ammoxidation activity

 $V_2O_5/CeF_3$  catalysts were prepared by wet impregnation method during which, the Cerium Vanadate (CeVO<sub>4</sub>) formation was observed and confirmed by pore size distribution, powder X-ray diffraction and FT-IR techniques. The CeVO<sub>4</sub> species is responsible for their high activity and selectivity for the ammoxidation of 3-picoline to nicotinonitrile

$$CH_3$$
  $+ O_2 + NH_3$   $- \frac{V_2O_5 / CeF_3}{300 - 410 \, ^{\circ}C}$   $+ 3 \, H_2O$   $+ 3 \, H_2O$ 

A.H. Padmasri, A. Venugopal, V. Siva Kumar, V. Shashikala, B.M. Nagaraja, P. Seetharamulu, B. Sreedhar, B. David Raju, P. Kanta Rao, K.S. Rama Rao

Journal of Molecular Catalysis A: Chemical 223 (2004) 329

Role of hydrotalcite precursors as supports for Pd catalysts in hydrodechlorination of CCl<sub>2</sub>F<sub>2</sub>

The selective synthesis of  $CH_2F_2$  by the hydrodechlorination of  $CCl_2F_2$  is studied over calcined Mg-Al and Mg-Cr hydrotalcites (CMA-HT & CMC-HT) supported Pd catalysts and their activities are compared with the corresponding oxides viz., MgO,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and  $Cr_2O_3$  supported Pd catalysts. Pd catalyst on the support from Mg-Al HT precursor is found to be superior and advantageous in terms of higher selectivity towards  $CH_2F_2$  formation and stability of the catalyst. Enhanced acidity of the used catalyst of Pd/CMA-HT compared to the fresh one manifested the higher selectivity towards  $CH_2F_2$ . The higher stability of Pd/CMA-HT can be attributed to the absence of any change in the surface Pd composition in the XPS analysis and the synergistic interaction of Pd with the support, calcined Mg-Al HT.

$$F \xrightarrow{Cl} Cl + 2H_2 \xrightarrow{Pd/Cal.Mg-AlHT} F + 2HCl$$

$$CFC-12 \qquad \qquad HFC-32$$

B.M. Nagaraja, V. Siva Kumar, V. Shashikala, A.H. Padmasri, S. Sreevardhan Reddy, B. David Raju, K.S. Rama Rao

Journal of Molecular Catalysis A: Chemical 223 (2004) 339

Effect of method of preparation of copper – magnesium oxide catalyst on the dehydrogenation of cyclohexanol

The superior catalytic activity of Cu/MgO co-precipitated catalyst in the dehydrogenation of cyclohexanol to cyclohexanone over corresponding impregnated and solid-solid wetting catalysts is ascribed to the higher Cu metal area and interaction between the micro-crystals of CuO and MgO associated with co-precipitated catalyst. Among the various coprecipitated Cu/MgO catalysts studied, the catalyst comprising of  $\sim$ 16wt.% Cu was found to show higher activity and selectivity towards the formation of cyclohexanone.

J. Krishna Murthy, S. Chandra Shekar, V. Siva Kumar, B. David Raju, B. Sreedhar, P.S. Sai Prasad, P. Kanta Rao, K.S. Rama Rao, F.J. Berry, L.E. Smart

Journal of Molecular Catalysis A: Chemical 223 (2004) 347

Effect of tungsten addition to Pd/ZrO<sub>2</sub> system in the hydrodechlorination activity of CCl<sub>2</sub>F<sub>2</sub>

The catalytic activity of Pd on W-ZrO $_2$  in the hydrodechlorination of  $CCl_2F_2$  was studied by varying  $WO_3$  content. Addition of tungsten to Pd/ZrO $_2$  system led to the formation of  $CHClF_2$  (HCFC-22) in the hydrodechlorination of  $CCl_2F_2$ . Thus the role of  $WO_3$  is to catalyze the partial dechlorination of  $CCl_2F_2$ . Absence of any structural changes of zirconia observed from XRD analysis indicates that these catalysts are highly resistant to the corrosive reaction atmosphere.

$$CCl_{2}F_{2} \xrightarrow[2H_{2}/\Delta]{} CHClF_{2} + HCl$$

$$CH_{2}F_{2} + 2HCl$$

$$Catalyst: Pd/WO_{3}-ZrO_{2}$$

Komandur V.R. Chary, Katar Sri Lakshmi, Pendyala Venkat Ramana Rao, Kamaraju Seetha Rama Rao, Maria Papadaki

Journal of Molecular Catalysis A: Chemical 223 (2004) 353

Characterization and catalytic properties of niobia supported nickel catalysts in the hydrodechlorination of 1,2,4-trichlorobenzene

Nickel supported on niobium oxide catalysts have been found to be highly active for the vapor phase hydrodechlorination of 1,2,4-trichlorobenzene. This paper deals with details characterization of nickel supported on niobia using XRD, XPS, TPR and hydrogen chemisorption. Further, these finding are related to catalytic properties during hydrodechlorination.

Komandur V.R. Chary, Kondakindi Rajender Reddy, Chinthala Praveen Kumar, Dhachapally Naresh, Vattikonda Venkat Rao, Gerhard Mestl

Journal of Molecular Catalysis A: Chemical 223 (2004) 363

Characterization and reactivity of molybdenum oxide catalysts supported on  $Nb_2O_5$ - $TiO_2$ 

The  ${\rm Nb_2O_5-TiO_2}$  mixed oxide is an interesting support to investigate the dispersion of molybdena and catalytic properties. Molybdena supported on Nb–Ti catalysts are found to be highly active and selective for the vapour phase ammoxidation of toluene to benzonitrile. This paper provides information on the surface species determined by various characterization techniques like oxygen chemisorption, XRD, TPR and LRS.