

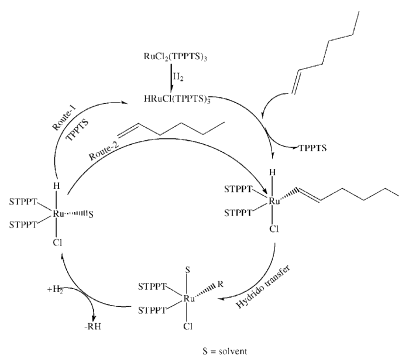
Contents

Articles

**Dharmesh U. Parmar, Sharad D. Bhatt,
Hari C. Bajaj, Raksh V. Jasra**

Journal of Molecular Catalysis A: Chemical
202 (2003) 9

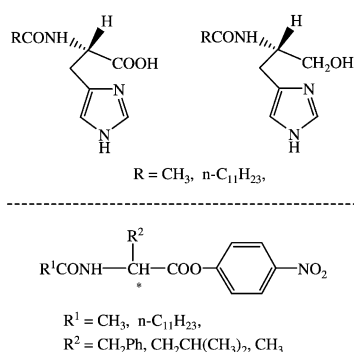
Hydrogenation of alkenes and aromatic
hydrocarbons using water-soluble RuCl_2
(TPPTS)₃ in aqueous medium



**Jing-Song You, Xiao-Qi Yu, Xiao-Yu Su,
Tao Wang, Qing-Xiang Xiang, Meng Yang,
Ru-Gang Xie**

Journal of Molecular Catalysis A: Chemical
202 (2003) 17

Hydrolytic metalloenzyme models. Enantio-
selective hydrolysis of long chain α -amino
acid esters by chiral metallomicelles com-
posed of lipophilic L-histidinol

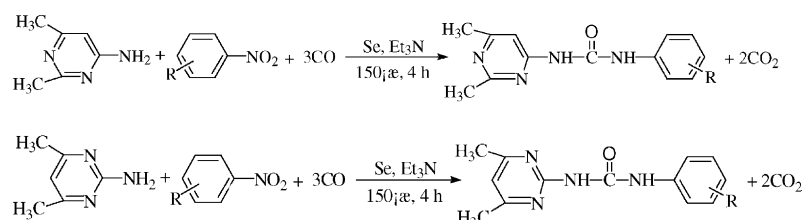


Gang Ling, Jinzhu Chen, Shiwei Lu

Journal of Molecular Catalysis A: Chemical
202 (2003) 23

Selenium-catalyzed carbonylation of substi-
tuted nitrobenzenes with aminomethyl-
pyrimidines as co-reagents to synthesize
N-phenyl-*N'*-methylpyrimidylurea derivatives

A series of *N*-phenyl-*N'*-methylpyrimidylurea derivatives have been synthesized via selenium-catalyzed reductive carbonylation of substituted nitrobenzenes with aminopyrimidine derivatives as co-reagents and carbon monoxide as carbonyl reagent.

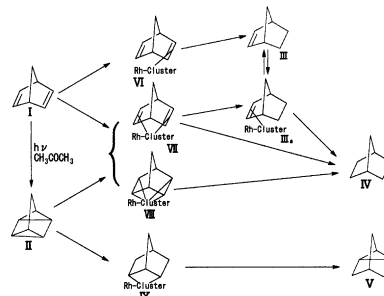


**Takanori Akioka, Yoshiharu Inoue,
Akihisa Yanagawa, Makoto Hiyamizu,
Yuzuru Takagi, Akira Sugimori**

Journal of Molecular Catalysis A: Chemical
202 (2003) 31

A comparative study on photocatalytic hydrogen transfer and catalytic hydrogenation of norbornadiene and quadricyclane catalyzed by $[\text{Rh}_6(\text{CO})_{16}]$

A comparative study on the hydrogenation of (I) and (II) were performed over photo-assisted activated $[\text{Rh}_6(\text{CO})_{16}]$ with or without UV-light irradiation. The photochemical and usual hydrogenations proceeded similarly as shown in reaction scheme.

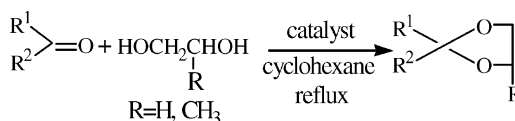


Shun-Jun Ji, Lin Wu

Journal of Molecular Catalysis A: Chemical
202 (2003) 41

Acetalization of carbonyl compounds catalyzed by polymer-bound metal complexes

A series of resin-bound metal complexes were prepared and characterized, their catalysis for acetalization of carbonyl compounds was examined.

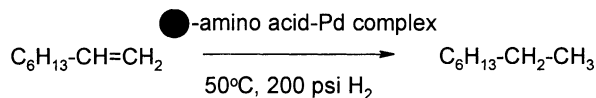


**Vaibhav B. Valodkar, Gopal L. Tembe,
Marayil Ravindranathan, R.N. Ram,
H.S. Rama**

Journal of Molecular Catalysis A: Chemical
202 (2003) 47

A study of synthesis, characterization and catalytic hydrogenation by polymer anchored Pd(II)-amino acid complexes

L-Valine was anchored to 6% and 8% cross-linked poly(styrene-divinyl benzene) resin and its complex with palladium chloride was prepared. The polymer supported Pd complexes behave as versatile and recyclable catalysts for the hydrogenation of 1-octene, cyclohexene, acetophenone and nitrobenzene. Kinetics of hydrogenation of 1-octene has been investigated in detail. The influence of different reaction parameters on conversion and selectivity to products are reported.

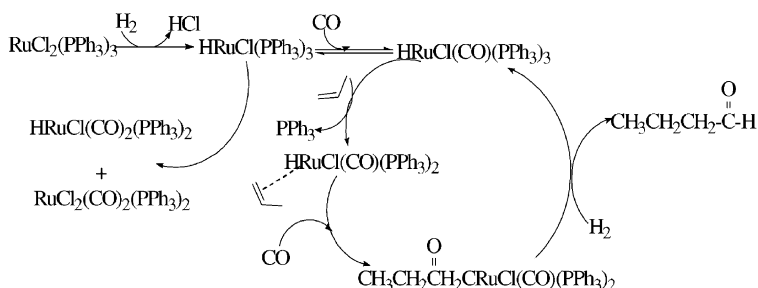


**Vivek K. Srivastava, Ram S. Shukla,
Hari C. Bajaj, Raksh V. Jasra**

Journal of Molecular Catalysis A: Chemical
202 (2003) 65

$\text{RuCl}_2(\text{PPh}_3)_3$ catalyzed liquid phase hydroformylation of propene under mild pressure conditions in alcoholic media: isolation and characterization of species separated out during the reaction

The low activity of $\text{RuCl}_2(\text{PPh}_3)_3$ catalyzed liquid phase hydroformylation of propene is attributed to the formation of in situ inactive $\text{HRuCl}(\text{CO})_2(\text{PPh}_3)_2$ and $\text{RuCl}_2(\text{CO})_2(\text{PPh}_3)_2$ intermediate complexes.

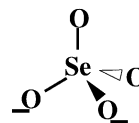


**Timothy T.Y. Tan, Donia Beydoun,
Rose Amal**

Journal of Molecular Catalysis A: Chemical
202 (2003) 73

Photocatalytic reduction of Se(VI) in aqueous solutions in UV/TiO₂ system: importance of optimum ratio of reactants on TiO₂ surface

This study investigates the effect of pH, initial solute concentrations on the UV/TiO₂ reduction of selenate ions. The adsorption of selenate and formate ions onto the TiO₂ surface was essential for selenate photoreduction. An interesting finding arisen from the current investigation is that the optimum reduction rate of selenate was closely correlated to the molar adsorption ratio of 3:1 of formate-to-selenate on the TiO₂ surface

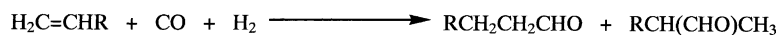
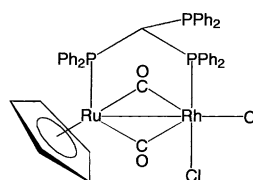


Maurice Abou Rida, Anthony K. Smith

Journal of Molecular Catalysis A: Chemical
202 (2003) 87

A bimetallic hydroformylation catalyst: high regioselectivity through heterobimetallic cooperativity

Heterobimetallic rhodium-ruthenium complexes exhibit a high regioselectivity in the hydroformylation reaction through cooperative effects. With the catalyst illustrated a ratio of 9:1 for linear versus branched aldehyde is obtained.

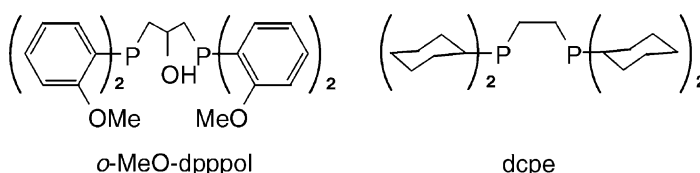


**Ingrid M. Angulo, Elisabeth Bouwman,
Remy van Gorkum, Sandra M. Lok,
Martín Lutz, Anthony L. Spek**

Journal of Molecular Catalysis A: Chemical
202 (2003) 97

New nickel-containing homogeneous hydrogenation catalysts. Structures of [Ni(*o*-MeO-dppol)Cl₂] and [Ni(dcpe)Cl₂]

The complexes [Ni(*o*-MeO-dppol)X₂] and [Ni(dcpe)X₂] (X = Cl, Br or I) have been synthesized and characterized using electronic absorption and IR spectroscopy. The X-ray structures of [Ni(*o*-MeO-dppol)Cl₂] and [Ni(dcpe)Cl₂] show the nickel ions to be in (distorted) square-planar geometries. The synthesized halide complexes and *in situ* mixtures of nickel acetate and the ligands were tested on catalytic activity in homogeneous hydrogenation. The ligand dcpe yields very active catalysts; turnover numbers up to 3000 in one hour have been obtained.

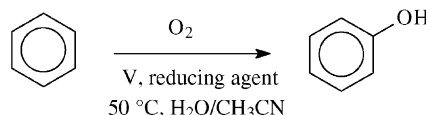


**Ezio Battistel, Roberto Tassinari,
Marco Fornaroli, Lucia Bonoldi**

Journal of Molecular Catalysis A: Chemical
202 (2003) 107

Oxidation of benzene by molecular oxygen catalysed by vanadium

Vanadium catalyses the oxidation of benzene to phenol with molecular oxygen in the presence of a reducing agent such as ascorbate (selectivity 98%). The effects of type of reducing agents and V ligands, as well as the solvent composition were studied. ESR measurements confirmed that V^{IV} species is rapidly formed in the reaction medium after the initial addition of V^{III}Cl₃ and explained qualitatively the time dependence of benzene oxidation.

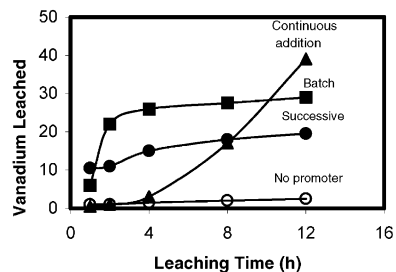


M. Marafi, A. Stanislaus

Journal of Molecular Catalysis A: Chemical
202 (2003) 117

Studies on rejuvenation of spent residue hydroprocessing catalysts by leaching of metal foulants

A comparative assessment of different modes of ferric nitrate addition to oxalic acid, namely, (i) continuous addition, (ii) batch addition, and (iii) successive addition, on the extraction of the deposited vanadium from the spent catalyst was studied to rejuvenate and reuse metal-fouled spent catalysts from residue hydroprocessing units. The continuous mode of addition of the reagent was more effective than the others in leaching vanadium and in recovering the surface area, pore volume and HDS activity of the catalyst.

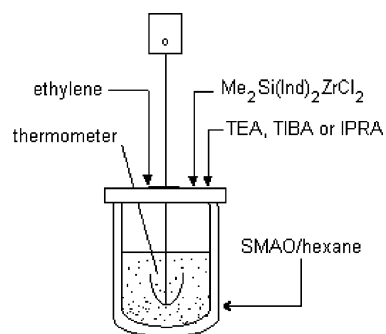


**Fernando C. Franceschini,
Tatiana T. da R. Tavares, Paula P. Greco,
Daniela Bianchini, Fernanda Chiarello
Stedile, Griselda B. Galland, João H.Z. dos
Santos, João B.P. Soares**

Journal of Molecular Catalysis A: Chemical
201 (2003) 127

Polypropylene obtained with in situ supported metallocene catalysts

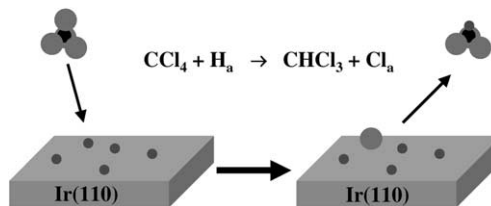
Propylene was polymerized by supported metallocene catalyst prepared by the in situ immobilization of $\text{Me}_2\text{Si}(\text{Ind})_2\text{ZrCl}_2$ on commercial MAO-modified silica (SMAO), using common alkylaluminum (TIBA, TEA or IPRA) as cocatalysts.

**C.T. Reeves, R.J. Meyer, C.B. Mullins**

Journal of Molecular Catalysis A: Chemical
202 (2003) 135

Dissociative adsorption and hydrodechlorination of CCl_4 on Ir(1 1 0)

The adsorption and hydrodechlorination of CCl_4 and other chlorinated methanes on Ir(1 1 0) were investigated. Adsorption of CCl_4 on the hydrogen precovered surface produces mainly CHCl_3 with trace amounts of CH_2Cl_2 and CH_4 . Similarly, adsorbed CHCl_3 will hydrodechlorinate to mainly CH_2Cl_2 . Hydrodechlorination of CCl_4 is favored at lower surface temperatures and at higher surface coverages of dissociatively adsorbed CCl_4 .

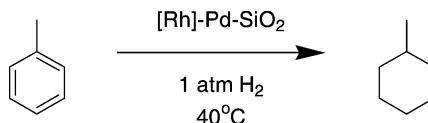


**Keith J. Stanger, Yali Tang,
James Anderegg, Robert J. Angelici**

Journal of Molecular Catalysis A: Chemical
202 (2003) 147

Arene hydrogenation using supported rhodium metal catalysts prepared from $[\text{Rh}(\text{COD})\text{H}]_4$, $[\text{Rh}(\text{COD})_2]^+\text{BF}_4^-$, and $[\text{Rh}(\text{COD})\text{Cl}]_2$ adsorbed on SiO_2 and Pd-SiO_2

The rhodium complexes, $[\text{Rh}(\text{COD})\text{H}]_4$, $[\text{Rh}(\text{COD})_2]^+\text{BF}_4^-$, $[\text{Rh}(\text{COD})\text{Cl}]_2$, and $\text{RhCl}_3 \cdot 3\text{H}_2\text{O}$, adsorbed on SiO_2 are optimally activated for toluene hydrogenation by pretreatment with H_2 at 200°C . The same complexes on Pd-SiO_2 are equally active without pretreatments. The active species in all cases is rhodium metal. The catalysts were characterized by XPS, TEM, DRIFTS, and mercury poisoning experiments.

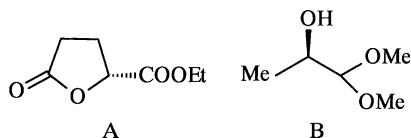


**Károly Felföldi, Katalin Balázsik,
Mihály Bartók**

Journal of Molecular Catalysis A: Chemical
202 (2003) 163

Heterogeneous asymmetric reactions. Part
32. High enantioselectivities in the hydroge-
nation of activated ketones on cinchona alka-
loid modified platinum-alumina catalysts

The enantioselective hydrogenation of the diethyl-2-oxoglutarate and pyruvaldehyde dimethyl acetal was investigated by cinchona alkaloid modified Pt-alumina catalysts. Under mild conditions an optical yield of 95–97% can be achieved. The products of the enantioselective hydrogenations, A and B, are valuable chiral building blocks.

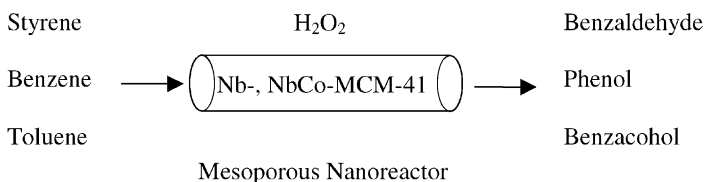


V. Parvulescu, C. Constantin, B.L. Su

Journal of Molecular Catalysis A: Chemical
202 (2003) 171

Liquid phase oxidation of aromatic hydro-
carbons using highly ordered Nb and NbCo-
MCM-41 nanoreactors

A series of highly ordered mesoporous Nb- and NbCo-containing silicas have been synthesized from sodium silicate or tetraethylortosilicate and characterized by various techniques. The very active oxidizing character of these catalysts was revealed in the liquid phase oxidation of styrene, benzene and toluene with H_2O_2 . A kinetic study was realized for oxidation of styrene with Nb-MCM-41 catalysts.

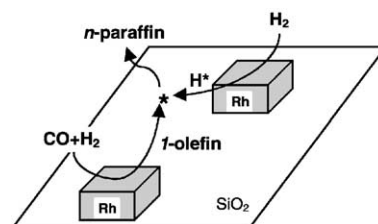


**M. Ojeda, M. López Granados, S. Rojas,
P. Terreros, J.L.G. Fierro**

Journal of Molecular Catalysis A: Chemical
202 (2003) 179

Influence of residual chloride ions in the CO
hydrogenation over Rh/SiO₂ catalysts

Silica-supported rhodium catalysts prepared from nitrate and chloride precursors were tested in the CO + H₂ reaction. The *ex*-chloride catalyst showed a lower 1-olefin/*n*-paraffin ratio. From the H₂-TPD results, it is suggested that residual chloride ions favour H₂-spillover from the Rh metal to the SiO₂ surface, thus leading to new active sites where olefins are hydrogenated to the corresponding paraffins.

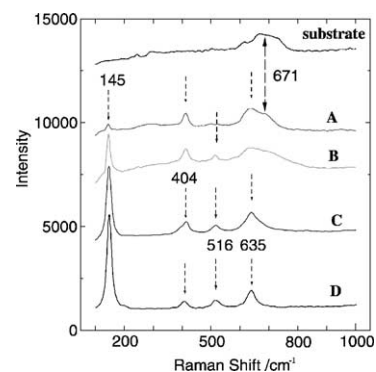


Jing Shang, Wei Li, Yongfa Zhu

Journal of Molecular Catalysis A: Chemical
202 (2003) 187

Structure and photocatalytic characteristics
of TiO₂ film photocatalyst coated on stainless
steel webnet

Raman spectra of (A) 50 nm thickness TiO₂ film; (B) 140 nm thickness TiO₂ film (C) 250 nm thickness TiO₂ film and (D) 360 nm thickness TiO₂ film. Substrate refers to the stainless steel webnet calcined at 400 °C for 10 min in an air flow oven. With increasing film thickness, anatase TiO₂ peaks (145, 404, 516 and 635 cm⁻¹) become more intense and the peak due to iron oxide (671 cm⁻¹) disappeared.

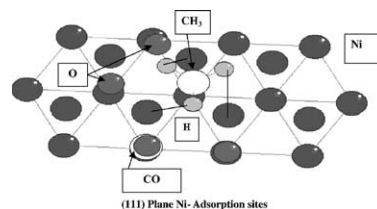


María Luján Ferreira, Nora N. Nichio, Osmar A. Ferretti

Journal of Molecular Catalysis A: Chemical 202 (2003) 197

A semiempirical theoretical study of Ni/ α -Al₂O₃ and NiSn/ α -Al₂O₃ catalysts for CH₄ reforming

A Molecular Orbital approach of the Extended Hückel type was performed to obtain the formation energies of postulated adsorbed and reacted forms of CH₄, H₂O, O₂ and CO₂ on a model of Ni and Ni-Sn surfaces, resembling Ni/ α -Al₂O₃ and Ni-Sn/ α -Al₂O₃. Three different known planes of fcc Ni were considered: (1 1 1), (0 0 1) and (1 1 0). Possible adsorbed and reacted CH₄, H₂O, O₂, CO₂ on Ni with Ni all around, Sn fully rounded by Ni and Ni near a Sn were discussed using reaction energies.

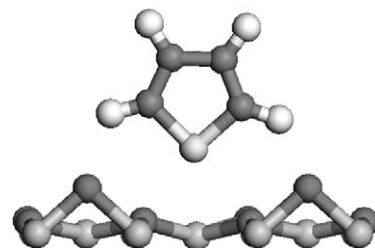


Gang Liu, José A. Rodriguez, Jan Hrbek, Brian T. Long, Donna A. Chen

Journal of Molecular Catalysis A: Chemical 202 (2003) 215

Interaction of thiophene with stoichiometric and reduced rutile TiO₂(1 1 0) surfaces: role of Ti³⁺ sites in desulfurization activity

The adsorption of thiophene on almost stoichiometric and defective TiO₂(1 1 0) surfaces was studied with photoemission spectroscopy, thermal desorption and density-functional slab calculations. Over an almost stoichiometric TiO₂(1 1 0) surface, the adsorption and desorption of thiophene are completely reversible. The orientation of the molecule changes as a function of coverage. Some C–S bond breaking was observed after introducing Ti³⁺ sites.

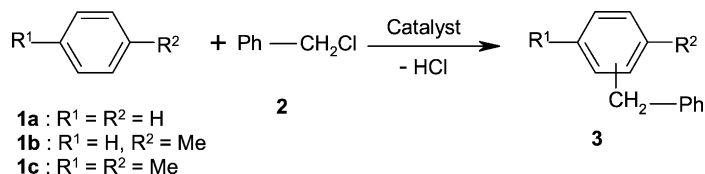


Ahmed Saber, Abdellatif Smahi, Abderrahim Solhy, Rachid Nazih, Brahim Elaabar, Mostapha Maizi, Saïd Sebti

Journal of Molecular Catalysis A: Chemical 202 (2003) 229

Heterogeneous catalysis of Friedel-Crafts alkylation by the fluorapatite alone and doped with metal halides

The fluorapatite (FAP) alone or doped with metal halide have been used as the new heterogeneous catalysts for the alkylation of benzene, toluene and *p*-xylene. The comparison of the activities of ZnCl₂, ZnBr₂, CuCl₂, CuBr₂ and NiCl₂ doped in FAP indicate that the best results were obtained with ZnCl₂/FAP and ZnBr₂/FAP. A high selectivity of monoalkyl compounds was observed in all cases.

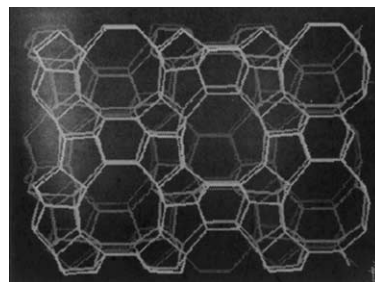


Jun Yang, Feng Deng, Mingjin Zhang, Qing Luo, Chaohui Ye

Journal of Molecular Catalysis A: Chemical 202 (2003) 239

W/HZSM-5 catalyst for methane dehydroaromatization: a multinuclear MAS NMR study

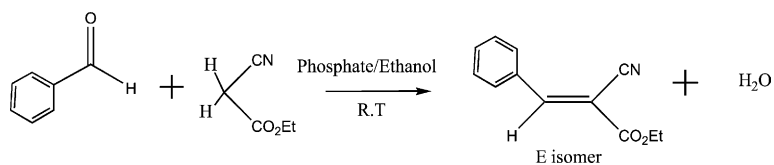
Multinuclear solid-state NMR techniques were employed to investigate the interaction between tungsten species and zeolite in W/HZSM-5 catalysts some of the W species disperse on the external surface and some of them diffuse into the internal channels of the zeolite, which causes a decrease of the Brønsted acid sites and silanols in the W/HZSM-5 catalysts. W⁴⁺ oxide acts as active metal sites for initial activation of methane on the W/HZSM-5 catalysts.



**Jamal Bennazha, Mohamed Zahouilly,
Ali Boukhari, Elizabeth M. Holt**

Journal of Molecular Catalysis A: Chemical
202 (2003) 247

Investigation of the basis of catalytic activity
of solid state phosphate complexes in the
Knoevenagel condensation

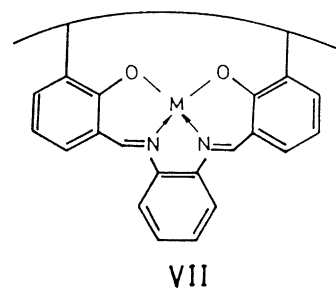


K.C. Gupta, H.K. Abdulkadir, S. Chand

Journal of Molecular Catalysis A: Chemical
202 (2003) 253

Synthesis of polymer anchored *N,N'*-bis(3-allyl salicylidene)-*o*-phenylenediamine cobalt (II) Schiff base complex and its catalytic activity for decomposition of hydrogen peroxide

N,N'-bis(3-Allyl salicylidene)-*o*-phenylenediamine cobalt(II) complex was heterogenized on new polymer support. The extent of cobalt(II) ions loading has been found to be a function of degree of cross-linking (Structure-VII). IR, UV and magnetic measurements confirmed the structure of cobalt (II) complex. The catalytic activity of heterogenized and homogenized cobalt(II) complex was evaluated taking decomposition of hydrogen peroxide as model reaction.

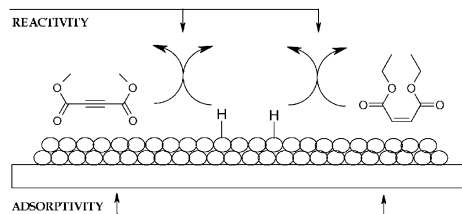


Petr Kačer, Petra Spurná, Libor Červený

Journal of Molecular Catalysis A: Chemical
202 (2003) 269

Coadsorption effect of the alkenic bond on the hydrogenation of the alkynic substrate on platinum and palladium catalysts

Competitive catalytic hydrogenation of dimethylester of acetylenecarboxylic acid, diethylester of fumaric acid and of maleic acid, respectively, were studied in liquid phase on palladium and platinum supported catalysts. Kinetic parameters evaluated from hydrogenation of individual substrates as well as of the binary systems in competitive arrangements allowed discussion of coadsorption effects of the alkenic bond on the hydrogenation course of the alkynic substrate.

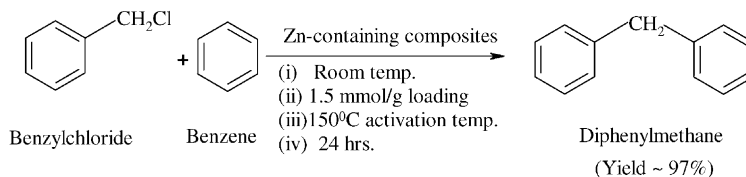


**Anjali Phukan, Jatindra Nath Ganguli,
Dipak Kumar Dutta**

Journal of Molecular Catalysis A: Chemical
202 (2003) 279

ZnCl₂-Zn²⁺-Montmorillonite composite: efficient solid acid catalyst for benzylation of benzene

A newer type of metal salt-metal ion exchanged Montmorillonite (Mont), MCl₂-Mⁿ⁺-Mont (M = Ni, Cu, Zn; n = 2) have been prepared and evaluated as solid acid catalysts for Friedel-Crafts reactions particularly for benzylation of benzene. The most efficient solid acid catalysts were found to be Zn-Mont containing composites.



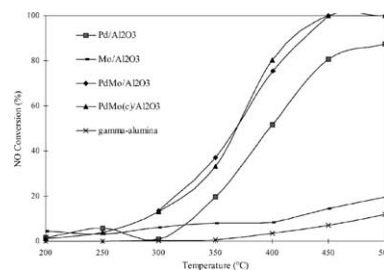
Zn-containing composites = Zn²⁺-Mont and
ZnCl₂-Zn²⁺-Mont

G.M. Tonetto, D.E. Damiani

Journal of Molecular Catalysis A: Chemical
202 (2003) 289

Performance of Pd-Mo/ γ -Al₂O₃ catalysts for the selective reduction of NO by methane

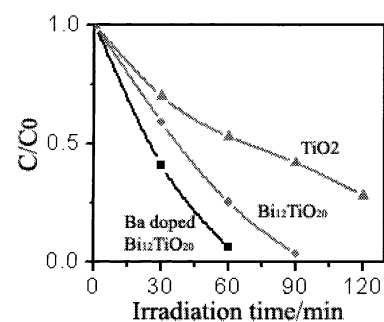
Selective catalytic reduction of NO by methane was studied on Pd-Mo/ γ -Al₂O₃ catalysts and was compared with corresponding monometallic catalysts. The activity for NO-CH₄ reaction was higher for the binary samples (200–500 °C). But a decrease in the activity (at 500 °C) was observed over the Pd-Mo/Al₂O₃ samples after 2 h under reaction conditions, being similar at the activity displayed by Pd/Al₂O₃.

**W. Feng Yao, Hong Wang, X. Hong Xu, Y. Zhang, X. Na Yang, S. Xia Shang, Y. Hui Liu, J. Tao Zhou, Min Wang**

Journal of Molecular Catalysis A: Chemical
202 (2003) 305

Characterization and photocatalytic properties of Ba doped Bi₁₂TiO₂₀

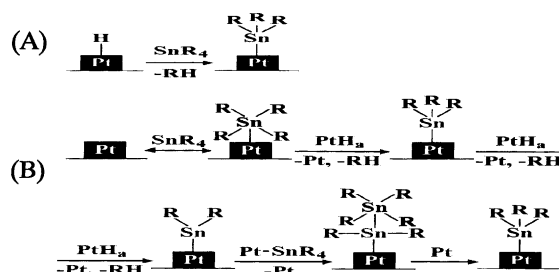
Doping of Bi₁₂TiO₂₀ with Ba ions was prepared by the chemical solution decomposition (CSD) method. Photocatalytic activities of the prepared samples were evaluated using methyl orange as a model organic compound. The result shows doping with 0.5 at. % Ba²⁺ can significantly increase the photoactivity of the Bi₁₂TiO₂₀ crystals.

**J.L. Margitfalvi, I. Borbáth**

Journal of Molecular Catalysis A: Chemical
202 (2003) 313

Time dependence of tin anchoring to supported platinum

Experimental evidences have been found supporting both (A) and (B) reaction pathways involved in tin anchoring into supported Pt.

**Ladislav Kurc, Marcel Páter, Libor Červený**

Journal of Molecular Catalysis A: Chemical
202 (2003) 327

Activity of basic catalysts in oxidation of 2-ethyl-5,6,7,8-tetrahydro-9,10-antrahydroquinone

Catalytic oxidation of 2-ethyl-5,6,7,8-tetrahydro-9,10-antrahydroquinone with oxygen was studied. This reaction is, as shown, specifically catalyzed by systems of a basic character, e.g. organic amines, basic heterogeneous catalysts, etc. The reaction rate is very sensitive to this parameter (basicity). Due to this fact the discussed oxidation was practically utilized as a basicity test reaction of the involved catalytic systems.

Special attention was paid to amines at their very low concentrations. The values of relative basicities for studies solutions of ethylamines in organic solvents were found to be different of those solved in water.

