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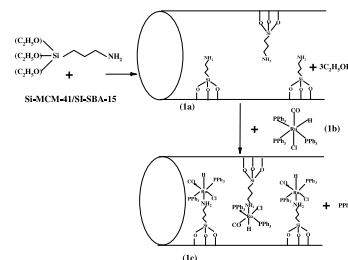
Articles

**Trissa Joseph, S.S. Deshpande,
S.B. Halligudi, A.Vinu, S. Ernst,
M. Hartmann**

Journal of Molecular Catalysis A: Chemical
206 (2003) 13

Hydrogenation of olefins over hydrido chloro-
carbonyl tris-(triphenylphosphine) rutheni-
um(II) complex immobilized on func-
tionized MCM-41 and SBA-15

Hydrido chlorocarbonyl tris-(triphenylphosphine) ruthenium(II) complex immobilized inside the pores of amine functionalized MCM-41 and SBA-15 materials were highly active in liquid phase hydrogenation of olefins than the neat complex catalyst. The catalyst immobilized in SBA-15 showed higher activity than MCM-41 in hydrogenation reaction.

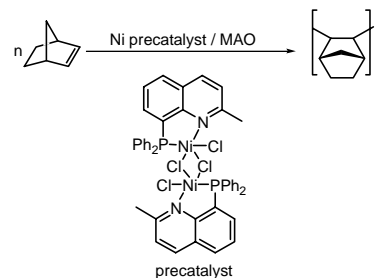


Haijian Yang, Zilong Li, Wen-Hua Sun

Journal of Molecular Catalysis A: Chemical
206 (2003) 23

Highly active vinyl-polymerization of norbornene by [2-methyl-8-(diphenylphosphino)quinoline]nickel(II) dichloride/methylaluminoxane

Vinyl-polymerization of norbornene was effectively promoted by highly active bis[2-methyl-8-(diphenylphosphino)quinoline]nickel dichloride/MAO catalytic system (activity $< 1.70 \times 10^8$ g-PNB/mol-Ni h). The catalytic activity and molecular weight and polydispersity of the resultant polymer can be controlled over a wide range by varying the reaction parameters.



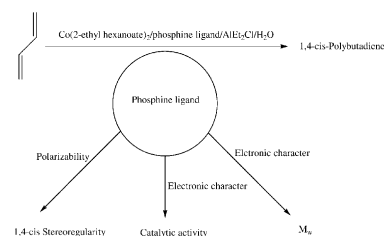
**Youngchan Jang, Pilsung Kim,
Ho Young Jeong, Hosull Lee**

Journal of Molecular Catalysis A: Chemical
206 (2003) 29

Effects of polarizability and electronic character of phosphine ligand on the polymerization of 1,3-butadiene using Co-based catalyst

The effects of phosphine ligands on the polymerization of 1,3-butadiene with $\text{Co}(\text{2-ethyl hexanoate})_2/\text{AlEt}_2\text{Cl}/\text{H}_2\text{O}$ were investigated. A good correlation was observed between the polarizability of phosphine ligands and 1,4-*cis* stereoregularity regardless of the electronic character (π -acceptor or σ -donor) of phosphine ligands. On the other hand, neither catalytic activity nor the molecular weight (M_w) of polybutadiene showed a good correlation with polarizability. Catalytic activity was affected only when phosphine ligands were inordinately strong π -acceptors and σ -donors, while the M_w of polybutadiene was

influenced significantly by the electronic character of phosphine ligands.

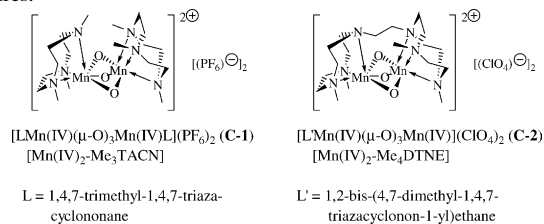


Vera Alves, Ewellyn Capanema,
Chen-Loung Chen, Josef Gratzl

Journal of Molecular Catalysis A: Chemical
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Comparative studies on oxidation of lignin
model compounds with hydrogen peroxide
using Mn(IV)-Me₃TACN and Mn(IV)-
Me₄DTNE as catalyst

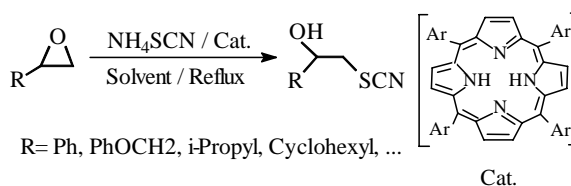
Figure illustrates the reaction mechanisms for the C-1- and C-2-catalyzed oxidation of the 1-(3,4-dimethoxyphenyl)ethanol (**1**), 1-(3,4-dimethoxyphenyl)-1-propene (**2**) and *E*-diphenylethene (**3**) with hydrogen peroxide. It also shows the pathways by which the oxidation products are produced from the substrates **1–3** on the basis of the kinetics and products identified in the reaction mixtures.



Hashem Sharghi, Mohammad Ali Nasser,
Alireza Hassani Nejad

Journal of Molecular Catalysis A: Chemical
206 (2003) 53

Efficient synthesis of β-hydroxy thiocyanates
from epoxides and ammonium thiocyanates
using tetraarylporphyrins as new catalysts

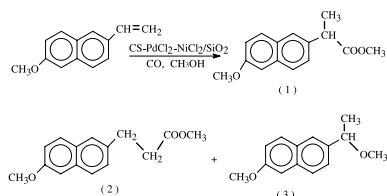


Jun Zhang, Chun-Gu Xia

Journal of Molecular Catalysis A: Chemical
206 (2003) 59

Natural biopolymer-supported bimetallic catalyst system for the carbonylation to esters of Naproxen

A silica-supported chitosan (CS)–palladium complex CS–PdCl₂/SiO₂ shows good conversion and higher regioselectivity in carbonylation of 6-methoxy-2-vinylnaphthalene. Effects of reaction variables have been studied to optimize reaction conditions. The hydroesterification of various substrates and the reuse of the catalyst were also investigated.

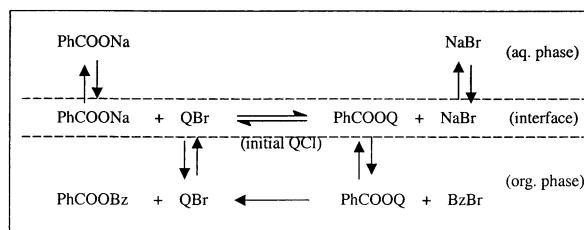


Hung-Ming Yang, Cheng-Liang Lin

Journal of Molecular Catalysis A: Chemical
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Phase-transfer catalyzed benzylation of sodium benzoate using aliquat 336 as catalyst in liquid–liquid system

The overall reaction and the reaction scheme are

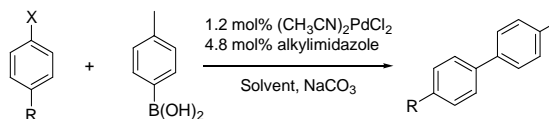


Christopher J. Mathews, Paul J. Smith, Tom Welton

Journal of Molecular Catalysis A: Chemical
206 (2003) 77

Novel palladium imidazole catalysts for Suzuki cross-coupling reactions

Commercially available alkylimidazoles generate palladium complexes that catalyse the Suzuki reaction.

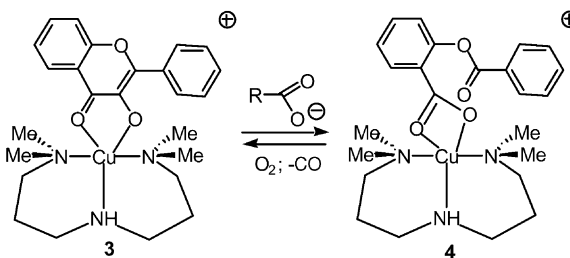


Éva Balogh-Hergovich, József Kaizer, Gábor Speier

Journal of Molecular Catalysis A: Chemical
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Carboxylate-enhanced reactivity in the oxygenation of copper flavonolate complexes

The rate of the oxygenolytic cleavage of flavonolate coordinated to copper(II) with the auxiliary ligand 3,3'-iminobis(*N,N*-dimethylpropylamine) is enhanced by the addition of carboxylate ligands.

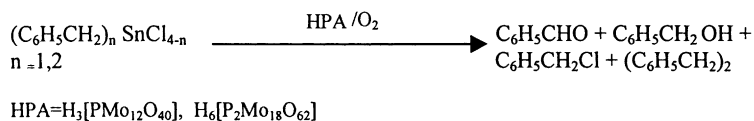


M.H. Alizadeh, H. Razavi, F.F. Bamoharram, K. Daneshvar

Journal of Molecular Catalysis A: Chemical
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The oxidative cleavage of carbon–tin bond catalyzed by heteropolyacids of molybdenum

The oxidation of organotin derivatives of dibenzylchlorotin and tribenzylchlorotin by dioxygen induced by $H_3[PMo_{12}O_{40}]$ and $H_6[P_2Mo_{18}O_{62}]$ have been investigated. Benzaldehyde is the main reaction product, accompanied by minor amounts of benzyl alcohol, benzyl chloride and dibenzyl. The effects of catalyst type, temperature and solvent on the reaction time have been examined.

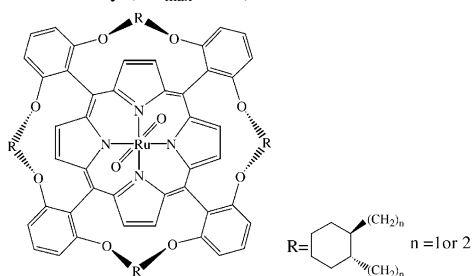


Paul Le Maux, Michel Lukas, Gérard Simonneaux

Journal of Molecular Catalysis A: Chemical
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New optically active ruthenium porphyrin catalysts for asymmetric epoxidation of styrenes

Two chiral ruthenium complexes have been used as enantioselective catalysts for the epoxidation of styrene derivatives using 2,6-dichloropyridine-*N*-oxide (Cl_2pyNO) as oxidant with moderate enantioselectivity (e.e._{max}: 35%).

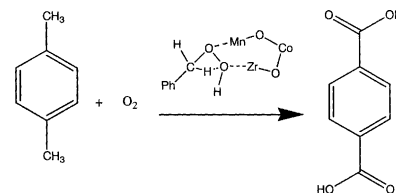


Walt Partenheimer

Journal of Molecular Catalysis A: Chemical
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The effect of zirconium in metal/bromide catalysts during the autoxidation of *p*-xylene Part I. Activation and changes in benzaldehyde intermediate formation

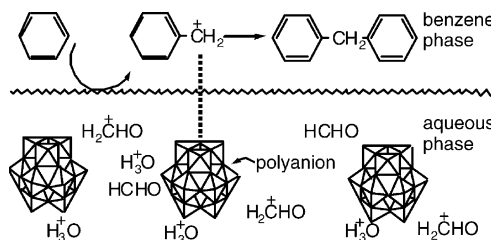
The changes in activity and intermediate formation by the addition of zirconium to a Co/Mn/Br and Co/Ce/Br catalyzed aerobic *p*-xylene oxidation are described. It is postulated that the benzyl hydroperoxide is dehydrated in the coordination sphere of the metals to give benzaldehyde and water and that the strong Lewis acidity of Zr(IV) is responsible for the experimental changes.

**Zhaoyin Hou, Toshio Okuhara**

Journal of Molecular Catalysis A: Chemical
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Condensation of benzene and aqueous formaldehyde to diphenylmethane in a biphasic system consisting of an aqueous phase of heteropolyacid

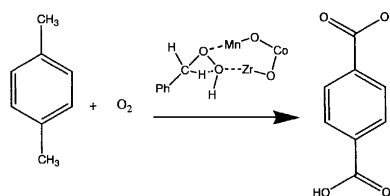
Heteropolyacids were highly active for the reaction of benzene with aqueous formaldehyde to diphenylmethane in a biphasic system. The critical reaction step is the attack by a benzyl cation to a benzene molecule, in which the intermediate benzyl cation is stabilized by heteropolyanion. The catalyst could be reused repeatedly without significant decrease in the activity.

**Walt Partenheimer**

Journal of Molecular Catalysis A: Chemical
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The effect of zirconium in metal/bromide catalysts on the autoxidation of *p*-xylene Part II. Alternative metals to zirconium and the effect of zirconium on manganese(IV) dioxide formation and precipitation with pyromellitic acid

Metals, such as Fe, V, Ti, Hf, have the same properties as Zr(IV), i.e. the ability to activate a Co/Mn/Br catalyst and to enhance the rate of benzaldehyde formation. Zr and Hf also have the ability to prevent manganese(IV) dioxide formation and carboxylic acid-metal precipitation. The unifying principle behind these phenomena are metals with high Lewis acidity.

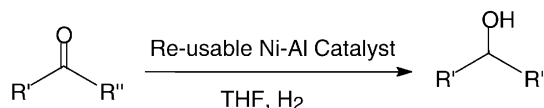


**Boyapati Manoranjan Choudary,
Mannepalli Lakshmi Kantam,
Ateeq Rahman,
Chinta Reddy Venkat Reddy**

Journal of Molecular Catalysis A: Chemical
206 (2003) 145

Selective reduction of aldehydes to alcohols by calcined Ni-Al hydrotalcite

Several aromatic and heterocyclic aldehydes are reduced at atmospheric pressure by calcined Ni-Al hydrotalcite and the catalyst is reused for several cycles with consistent activity and selectivity.



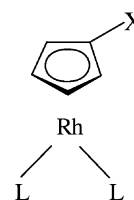
**Luigi Busetto, M. Cristina Cassani,
Rita Mazzoni, Piero Frediani,
Eleonora Rivalta**

Journal of Molecular Catalysis A: Chemical
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Hydroformylation of olefins catalysed by
alkoxycarbonylcyclopentadienyl complexes
of rhodium(I)

The hydroformylation of 1-hexene and styrene
with syngas (30 bar of 1:1 CO/H₂) in the
presence of the alkoxycarbonylcyclopentadienyl
rhodium(I) complexes [Rh{C₅H₄CO₂X
(L,L)}] [X = -CH₂CH=CH₂, -(CHR)₂OH
(R=H, Me); L,L=2CO, NBD] has been studied
and compared with the unsubstituted system
[Rh(C₅H₅)NBD]. L,L=NBD, X=-CO₂CH₂-
CH₂OH (1); L,L=2CO, X=-CO₂-CH₂-
CH₂OH (2); L,L=2CO, X=-CO₂CH₂-
CH=CH₂ (3); L,L=NBD, X=(dl)-CO₂CH

(Me)CH(Me)OH (4); L,L=NBD, X = (S,S)-
CO₂CH(Me)CH(Me)OH (5); L,L= NBD,
X=H (6).

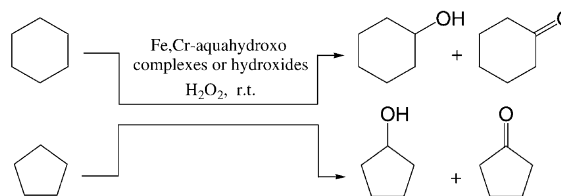


**M.N. Kopylovich, A.M. Kirillov,
A.K. Baev, A.J.L. Pombeiro**

Journal of Molecular Catalysis A: Chemical
206 (2003) 163

Heteronuclear iron(III)–chromium(III) hydroxo
complexes and hydroxides, and their
catalytic activity towards peroxidative oxidation
of alkanes

Relations between the catalytic activity of Fe(III)–Cr(III) aquahydroxo complexes or hydroxides and their compositions towards peroxidative oxidation of cyclohexane and cyclopentane to the corresponding ketones and alcohols were recognised, and a *synergic effect* was detected for the mixed (heteronuclear) hydroxides in the cyclohexane oxidation.

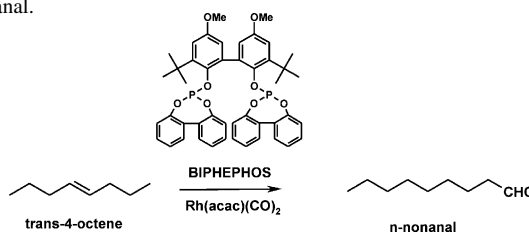


**Arno Behr, Dietmar Obst,
Christian Schulte, Thorsten Schosser**

Journal of Molecular Catalysis A: Chemical
206 (2003) 179

Highly selective tandem isomerization–
hydroformylation reaction of *trans*-4-octene
to *n*-nonanal with rhodium-BIPHEPHOS
catalysis

The hydroformylation of the internal olefin *trans*-4-octene to *n*-nonanal using the solvent toluene could be carried out with good yields of 89%. At a temperature of 125 °C the reaction proved to be very fast (4 h, TOF = 46 h⁻¹) and very selective. Performing the reaction in propylene carbonate reveals a significant influence on the selectivity, ending up to a value of 95% of *n*-nonanal.

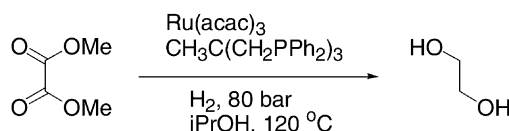


**Marcel Chr. van Engelen, Herman T.
Teunissen, Johannes G. de Vries,
Cornelis J. Elsevier**

Journal of Molecular Catalysis A: Chemical
206 (2003) 185

Suitable ligands for homogeneous ruthenium-catalyzed hydrogenolysis of esters

A catalytic system for the hydrogenolysis of dimethyl oxalate to ethylene glycol has been obtained in situ from Ru(acac)₃ with the facially coordinating tridentate phosphine ligand CH₃C(CH₂PPh₂)₃. This catalyst enabled full and selective conversion and is far more active than the known homogeneous catalysts able to hydrogenate dimethyl oxalate to ethylene glycol. When using the meridional coordinating ligand PhP(C₂H₄PPh₂)₂, selectivity can be directed toward the semi-hydrogenolysis product methyl glycolate.

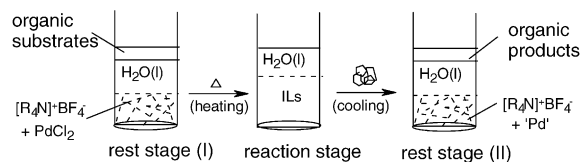


**Gang Zou, Zhiyong Wang, Junru Zhu,
Jie Tang, Ming Y. He**

Journal of Molecular Catalysis A: Chemical
206 (2003) 193

Developing an ionic medium for ligandless-palladium-catalysed Suzuki and Heck couplings

Alkylammonium tetrafluoroborates melt in water at much lower temperatures than their normal melting points to form an aqueous-ionic liquid biphasic system, thus can serve as a green liquid medium for ligandless-palladium-catalysed C–C bond-forming couplings during the reaction stage and be readily separated and purified in the solid state by recrystallization during the rest stages.

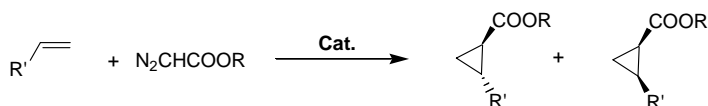


Hongwang Wang, Wei Sun, Chungu Xia

Journal of Molecular Catalysis A: Chemical
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An easily recoverable and efficient catalyst for heterogeneous cyclopropanation of olefins

The cyclopropanation reactions between olefins and diazoacetates were catalyzed by chitosan-Schiff base copper complexes to give high yields and moderate enantioselectivities. The catalyst could be recovered and reused.

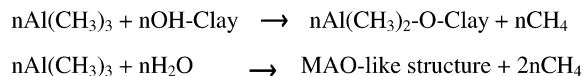


**Dong Wook Jeong, Dae Sik Hong,
Hyun Yong Cho, Seong Ihl Woo**

Journal of Molecular Catalysis A: Chemical
206 (2003) 205

The effect of water and acidity of the clay for ethylene polymerization over Cp₂ZrCl₂ supported on TMA-modified clay materials

The organic aluminum compounds (OACs) have been prepared on the surface of clay such as montmorillonite K-10 (MMT-10) and Kunipia by reaction of partial hydrolysis of trimethylaluminum (TMA). The effect of water and acidity of the clay in ethylene polymerization was investigated over Cp₂ZrCl₂ supported on the TMA-modified clay.

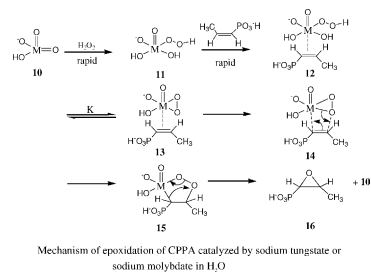


**Xin-Yan Wang, Hong-Chang Shi,
Shou-Yi Xu**

Journal of Molecular Catalysis A: Chemical
206 (2003) 213

Kinetics and mechanism on the epoxidation of *cis*-1-propenylphosphonic acid in H₂O catalyzed by tungstate(VI) or molybdate(VI)

Epoxidation of *cis*-1-propenylphosphonic acid (CPPA) was carried out using Na₂WO₄ or Na₂MoO₄ as catalysts in H₂O. A mechanism of epoxidation was suggested and discussed from the kinetic and IR study. The research indicated that not only in non-protic solvents but also in H₂O, the active peroxy groups were the metal-dioxygen rings in the epoxidation of olefins catalyzed by W(VI) or Mo(VI) compounds.

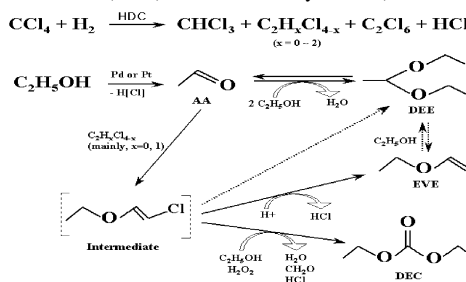


**Jong Wook Bae, Eun Joo Jang,
Dong Hyun Jo, Jae Sung Lee**

Journal of Molecular Catalysis A: Chemical
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Liquid-phase hydrodechlorination of CCl_4 in a medium of ethanol with co-production of acetal and diethyl carbonate

Liquid-phase hydrodechlorination (HDC) of CCl_4 over supported Pd or Pt catalysts in the presence of $\text{C}_2\text{H}_5\text{OH}$ gave not only the selective synthesis of CHCl_3 , but also conversion of $\text{C}_2\text{H}_5\text{OH}$ to diethyl carbonate (DEC) and 1,1-diethoxyethane (acetal; DEE).

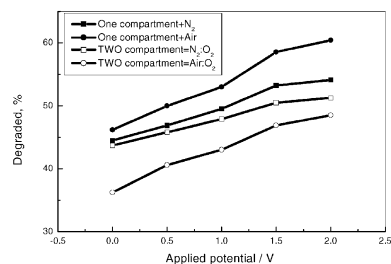


W.H. Leng, Z. Zhang, J.Q. Zhang

Journal of Molecular Catalysis A: Chemical
206 (2003) 239

Photoelectrocatalytic degradation of aniline over rutile TiO_2/Ti electrode thermally formed at 600°C

The photoelectrochemical oxidation of aniline on rutile form TiO_2 film electrodes was studied both in single and double compartment photoreactors, and the role of oxygen, applied potential were discussed simultaneously. The results showed that the rutile form of TiO_2/Ti electrode had excellent photoactivity by applying anodic bias potential and irradiation simultaneously.

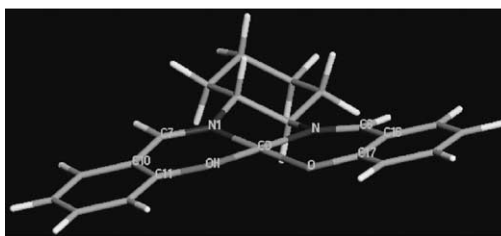


**Eugen Möllmann, Petra Tomlinson,
W.F. Hölderich**

Journal of Molecular Catalysis A: Chemical
206 (2003) 253

Demonstration of a zeolite effect on an encapsulated Co-salen-complex

Extensive molecular dynamics simulations of a Co-salen-complex captured inside a zeolite matrix showed, that due to the zeolite the complex prefers a distorted conformation which is preserved in course of the simulations at different temperatures and that the zeolite is able to confine the occluded complex to this conformation even at higher temperatures.

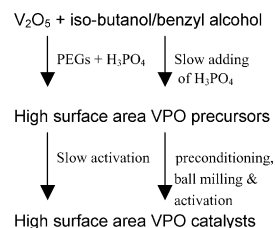


**Xiaoshu Wang, Lijun Xu, Xi Chen,
Weijie Ji, Qijie Yan, Yi Chen**

Journal of Molecular Catalysis A: Chemical
206 (2003) 261

Novel modifications in preparing vanadium phosphorus oxides and their applications for partial oxidation of *n*-butane

A successful approach to preparing high surface area VPO system by using PEGs as the unique additive has been established. Another approach to preparing high surface area VPO, namely, well-controlled addition of phosphoric acid to generate a high surface area VPO precursor, short pre-conditioning of the precursor and final ball the as-treated precursor, was also set up. The resulting materials showed notably enhanced performances.

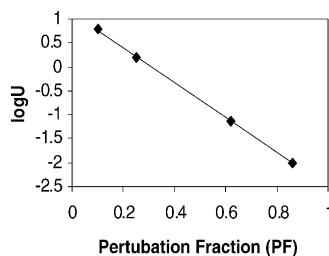


Ralph A. Gardner-Chavis, John Reye

Journal of Molecular Catalysis A: Chemical
206 (2003) 269

Unified explanation of catalyzed and non-catalyzed chemical reactions

Atomic Energy Levels (AEL) tables, from NIST, are used to determine a catalyst for a reaction. Gaseous reactants are perturbed to react by an electric field with a fractional charge.



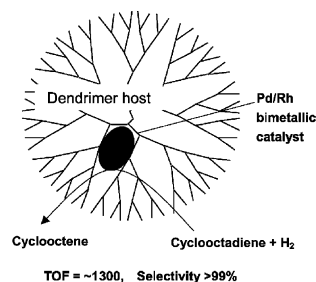
PF	Metal Ion	U	Log U
0.1	III Cr	6.144	0.788
0.25	II Fe	1.552	0.191
0.62	II Co	0.074	-1.131
0.86	III Ni	0.01	-2.000

Young-Min Chung, Hyun-Ku Rhee

Journal of Molecular Catalysis A: Chemical
206 (2003) 291

Partial hydrogenation of 1,3-cyclooctadiene using dendrimer-encapsulated Pd–Rh bimetallic nanoparticles

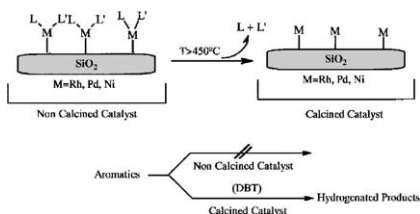
Dendrimer-encapsulated Pd–Rh bimetallic nanoparticles show a promising catalytic activity in partial hydrogenation of 1,3-cyclooctadiene.

**S. Rojas, P. Terreros, M.A. Peña, M. Ojeda, J.L.G. Fierro, A. Otero, F. Carrillo**

Journal of Molecular Catalysis A: Chemical
206 (2003) 299

Hydrogenation of aromatics over supported noble metal catalysts ex organometallic complexes

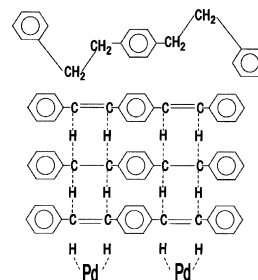
A number of organometallic complexes have been anchored onto both SiO₂ and silylated-SiO₂ carriers. The solids have been tested in the aromatic hydrogenation reaction operating at high temperatures and pressures. The performance of the catalysts operating under sulphur rich environments has also been explored. The solids were found active on the HDA reaction once the ligands were removed out of the metallic function.

**Ilan Pri-Bar, Jacob E. Koresh**

Journal of Molecular Catalysis A: Chemical
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Supramolecular selectivity in solid phase catalytic hydrogenation of phenylalkynyl and azobenzene derivatives

The mechanism of Palladium catalyzed hydrogenation in solid phase of phenylalkynyl and azobenzene derivatives is found to consist of supramolecular selective hydrogenation of assemblies of unsaturated substrate molecules on metallic catalyst.

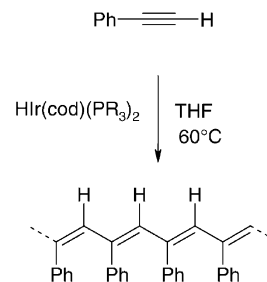


**Mauro Marigo, Dunja Millos,
Nazario Marsich, Erica Farnetti**

Journal of Molecular Catalysis A: Chemical
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Iridium-catalyzed formation of *trans*-poly-phenylacetylene by alkyne polymerization

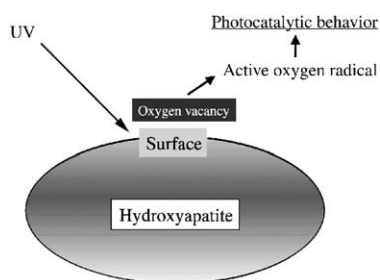
The compounds $\text{HIr}(\text{cod})(\text{PR}_3)_2$ (cod: 1,5-cyclooctadiene; PR_3 : PPh_3 , $\text{P}(p\text{-MeOC}_6\text{H}_4)_3$, $\text{P}(o\text{-MeOC}_6\text{H}_4)_2$, PCyPh_2) catalyze the polymerization of phenylacetylene (PA) to give *trans*-polyphenylacetylene (PPA). The catalytic reactions are highly stereoselective, and produce only small amounts of oligomeric products. From the catalytic mixtures the iridium(III) derivatives *fac*- $\text{HIr}(\text{C}\equiv\text{CPh})_2(\text{PR}_3)_3$ were isolated. Spectroscopic studies provide information on the evolution of the iridium precursors during the catalytic reaction.



Harumitsu Nishikawa

Journal of Molecular Catalysis A: Chemical
206 (2003) 331

Surface changes and radical formation on hydroxyapatite by UV irradiation for inducing photocatalytic activation

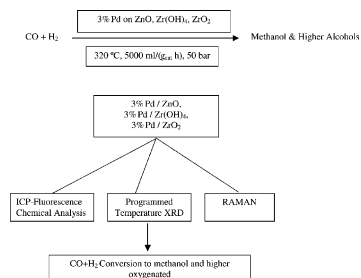


**M. Josefina Pérez-Zurita,
Michelle Cifarelli, M. Luisa Cubeiro,
Juan Alvarez, Mireya Goldwasser,
Egle Pietri, Luis Garcia,
Antoine Aboukais,
Jean-François Lamonier**

Journal of Molecular Catalysis A: Chemical
206 (2003) 339

Palladium-based catalysts for the synthesis of alcohols

The present work intends to illustrate the effects of precursor and support composition on the structure and performance of Pd-based catalysts for the synthesis of methanol and higher oxygenated compounds. The power of the XRD technique and the reaction itself, as characterisation tools, was evidenced.

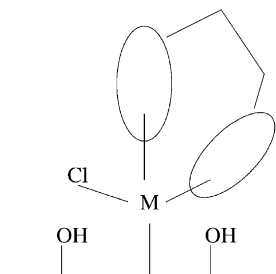


**Rafael Guimarães, Fernanda C. Stedile,
João H.Z. dos Santos**

Journal of Molecular Catalysis A: Chemical
206 (2003) 353

Ethylene polymerization with catalyst systems based on supported metallocenes with varying steric hindrance

A series of metallocenes differing in the metal center ($M = \text{Zr}, \text{Ti}, \text{Hf}$), in the coordination sphere (RCp , with $R = \text{H}, \text{Me}, i\text{Bu}, n\text{Bu}$; Indenyl) and the bridge ($\text{Et}, \text{Me}_2\text{Si}$) were studied as homogeneous systems and supported on silica and MAO-mediated (2wt.% Al/SiO_2) silica. The effect of these parameters were evaluated in the grafted metal content, in catalyst activity and in polymer properties.

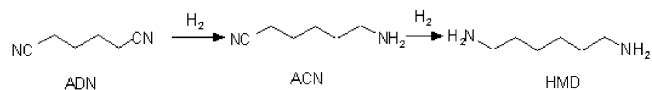


**S. Alini, A. Bottino, G. Capannelli,
R. Carbone, A. Comite, G. Vitulli**

Journal of Molecular Catalysis A: Chemical
206 (2003) 363

The catalytic hydrogenation of adiponitrile to hexamethylenediamine over a rhodium/alumina catalyst in a three phase slurry reactor

Adiponitrile was hydrogenated to hexamethylenediamine (HMD) in a three phase slurry reactor at 353K and 3MPa using Rh/Al₂O₃. Comparisons were made with a Raney Ni catalyst currently used in the industrial production of HMD. The influence of temperature and pressure on both conversion and selectivity was investigated. The rhodium based catalyst provided good adiponitrile conversion and HMD selectivity. The Rh/Al₂O₃ catalyst was prepared using the Metal Vapour Synthesis Technique.

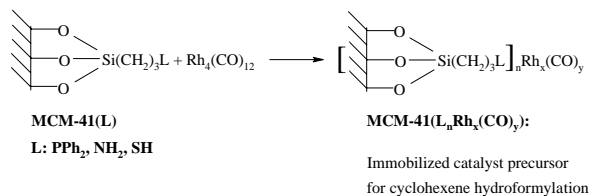


L. Huang, J.C. Wu, S. Kawi

Journal of Molecular Catalysis A: Chemical
206 (2003) 371

Rh₄(CO)₁₂-derived functionalized MCM-41-tethered rhodium complexes: preparation, characterization and catalysis for cyclohexene hydroformylation

Rh₄(CO)₁₂-derived rhodium carbonyls are tethered to MCM-41(PPh₂), MCM-41(NH₂) and MCM-41(SH) which are formed by functionalization of silicate MCM-41 with phosphine, amine and thiol ligands. The MCM-41(NH₂)-tethered rhodium carbonyl catalyst is of advantage in activity and stability over the MCM-41(PPh₂)- and MCM-41(SH)-tethered ones in cyclohexene hydroformylation.

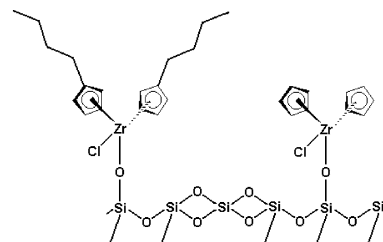


**Fernando Silveira, Silvia R. Loureiro,
Griselda B. de Galland,
Fernanda C. Stedile,
João Henrique Z. dos Santos,
Toshiharu Teranishi**

Journal of Molecular Catalysis A: Chemical
206 (2003) 389

Hybrid zirconocene supported catalysts

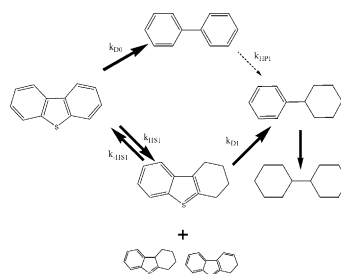
A series of supported catalysts were prepared by combining (*n*BuCp)₂ZrCl₂ and Cp₂ZrCl₂ sequentially grafted on silica in different ratios (1:1 and 1:3) and immobilization order. Catalyst activity was shown to be dependent on the metallocene nature, but not on the addition order or on molar ratio.



**Hamdy Farag, Kinya Sakanishi,
Masato Kouzu, Akimitsu Matsumura,
Yoshikazu Sugimoto, Ikuo Saito**

Journal of Molecular Catalysis A: Chemical
206 (2003) 399

Dibenzothiophene hydrodesulfurization over synthesized MoS₂ catalysts

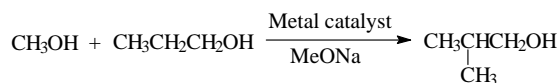


**Carlo Carlini, Alessandro Macinai,
Mario Marchionna, Marilena Noviello,
Anna Maria Raspolli Galletti,
Glaucio Sbrana**

Journal of Molecular Catalysis A: Chemical
206 (2003) 409

Selective synthesis of isobutanol by means of the Guerbet reaction. Part 3: Methanol/*n*-propanol condensation by using bifunctional catalytic systems based on nickel, rhodium and ruthenium species with basic components

The catalytic synthesis of isobutanol via the Guerbet condensation of methanol with *n*-propanol, has been studied. Bifunctional catalysts based on either heterogeneous or homogeneous dehydrogenating/hydrogenating nickel (rhodium or ruthenium) species combined with sodium methoxide as basic component were investigated.

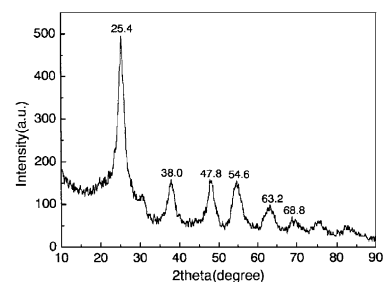


Yibing Xie, Chunwei Yuan

Journal of Molecular Catalysis A: Chemical
206 (2003) 419

Photocatalytic activity and recycle application of titanium dioxide sol for X-3B photodegradation

Titanium dioxide sol nanoparticles, prepared under low temperature (62°C) and ambient pressure, show pure anatase crystalline structure due to presence of attributive diffraction peaks ($2\theta = 25.4^\circ, 38.0^\circ, 47.8^\circ$). This property contributes to its photocatalytic activity of TiO₂ hydrosol for dye photodegradation under visible light irradiation.

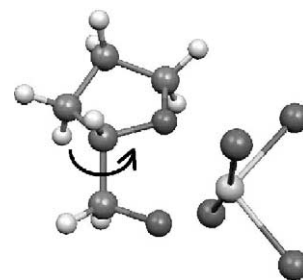


Zygmunt Flisak, Krzysztof Szczegot

Journal of Molecular Catalysis A: Chemical
206 (2003) 429

DFT analysis of titanium complexes with oxygen-containing bidentate ligands

Strength of the Ti–O bonds in titanium complexes with certain oxygen-containing bidentate ligands has been investigated by means of DFT. Formation of complexes with monodentate dangling ligands has also been discussed.



**D.J. Thompson, M.O. Fanning,
B.K. Hodnett**

Journal of Molecular Catalysis A: Chemical
206 (2003) 435

The interplay of electrostatic and covalent effects in 1-butene oxidation over vanadyl pyrophosphate

