

## Contents

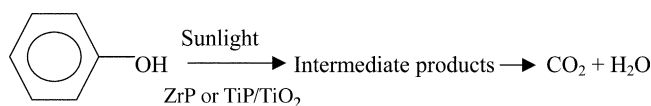
### Articles

**Dipti Prakasini Das, Kulamani Parida,  
Bhudev Ranjan De**

*Journal of Molecular Catalysis A: Chemical 240*  
(2005) 1

Photo-oxidation of phenol over titania pillared  
zirconium phosphate and titanium phosphate

The photocatalytic degradation of phenol under solar radiation depends on surface area, basal spacing and acid sites present in titania pillared ZrP and TiP. Two weight percent titania loaded ZrP and 4 wt% titania loaded TiP show highest phenol degradation compared to other loaded samples of ZrP and TiP. Complete phenol degradation (10mg/L) took place at pH 6.0 in 4 h with 0.6g/L catalyst under solar radiation.

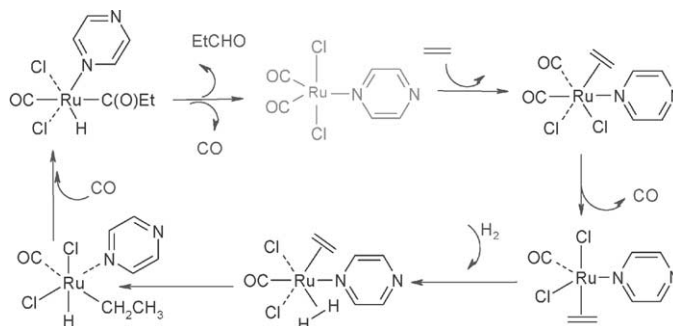


**M.A. Moreno, M. Haukka, A. Turunen,  
T.A. Pakkanen**

*Journal of Molecular Catalysis A: Chemical 240*  
(2005) 7

Monomeric ruthenium carbonyls containing  
2-substituted pyrazines  
From synthesis to catalytic activity in 1-hexene  
hydroformylation

Ru–pyrazine complexes show good activities for the hydroformylation of 1-hexene. The catalysts activates via *cis*-decarbonylation of the original hexacoordinated [Ru(CO)<sub>3</sub>Cl<sub>2</sub>(pz)] producing the necessary vacancy required for coordination of the substrates.

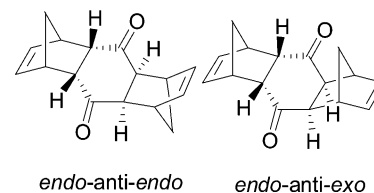


**M. Victoria Gómez, Ángel Cantín,  
Avelino Corma, Antonio de la Hoz**

*Journal of Molecular Catalysis A: Chemical 240*  
(2005) 16

Use of different microporous and mesoporous  
materials as catalyst in the Diels Alder and  
Retro-Diels Alder reaction between cyclopenta-  
diene and *p*-benzoquinone. Activity of Al-, Ti- and  
Sn-doped silica

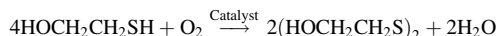
Diels–Alder cycloaddition has been studied using  
amorphous silica and different ITQ-2 and MCM-  
41 pure silica and metal containing materials as  
catalysts. The introduction of transition metal  
atoms in the framework increases the reaction rate  
preserving the selectivity to the *endo-endo* isomer.  
The presence of acidic OH groups provoke the  
retro-Diels–Alder reaction increasing the selectiv-  
ity to the *endo-exo* isomer.



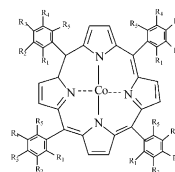
M. Hassanein, S. Gerges, M. Abdo,  
S. El-Khalafy

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 22

Catalytic activity and stability of anionic and cationic water soluble cobalt(II) tetraarylporphyrin complexes in the oxidation of 2-mercaptoethanol by molecular oxygen



Catalyst:



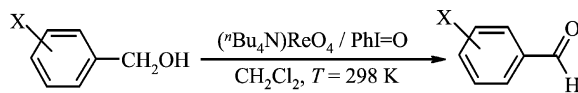
	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>
1	Cl	SO <sub>3</sub> Na	H	H	Cl
2	CH <sub>3</sub>	SO <sub>3</sub> Na	CH <sub>3</sub>	SO <sub>3</sub> Na	CH <sub>3</sub>
3	H	H	N <sup>+</sup> (Et) <sub>2</sub> Me <sup>-</sup>	H	H

Patrina Paraskevopoulou, Nikos Psaroudakis,  
Spyros Koinis, Pericles Stavropoulos,  
Konstantinos Mertis

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 27

Catalytic selective oxidation of benzyl alcohols to aldehydes with rhenium complexes

The system (<sup>n</sup>Bu<sub>4</sub>N)ReO<sub>4</sub>/PhIO catalyses effectively in organic media and under mild conditions the selective oxidation of primary benzyl alcohols to the corresponding aldehydes; in contrast, it is inactive towards a range of secondary benzyl alcohols and aliphatic (primary and secondary) alcohols.

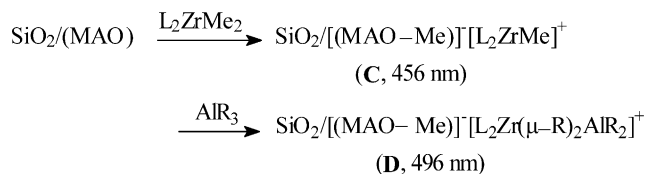


V.N. Panchenko, V.A. Zakharov, E.A. Paukshtis

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 33

Study of the supported zirconocene catalysts by means of UV/vis and DRIFT spectroscopy

Various types of the surface zirconocene species [(C) and (D) in the scheme below and [Me<sub>2</sub>Si(Ind)<sub>2</sub>ZrCl]<sup>+</sup>[MeMAO]<sup>-</sup> (E)] are identified in the supported catalysts Me<sub>2</sub>Si(Ind)<sub>2</sub>ZrX<sub>2</sub>/MAO/SiO<sub>2</sub> (X=Cl, Me) by means of UV/vis in diffusion reflection mode (DRS) and DRIFT spectroscopy. It is shown the species of (D) type are formed only at the interaction of the supported catalysts with TIBA.

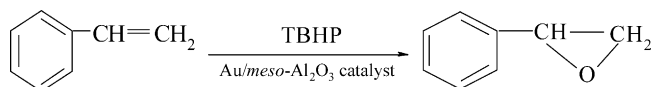


Donghong Yin, Liangsheng Qin, Jianfu Liu,  
Chengyong Li, Yong Jin

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 40

Gold nanoparticles deposited on mesoporous alumina for epoxidation of styrene: Effects of the surface basicity of the supports

Nanometer Au particles deposited on different supports of mesoporous Al<sub>2</sub>O<sub>3</sub> via HDP method used as highly active/selective and reusable catalysts for epoxidation of styrene. The dispersion and average size of the gold particles are dependent of the number of surface basic sites on the supports.

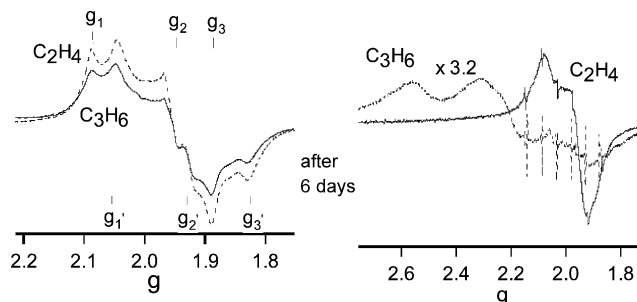


**Saburo Hosokawa, Yuko Fujinami,  
Hiroyoshi Kanai**

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 49

Reactivity of Ru=O species in RuO<sub>2</sub>/CeO<sub>2</sub> catalysts prepared by a wet reduction method

The calcination of RuO<sub>2</sub>/CeO<sub>2</sub> prepared by a wet reduction method produced Ru=O bonds, which were enhanced by heating in O<sub>2</sub>. The ESR study revealed that the Ru=O bonds discriminated between their reactivity with propylene and ethylene. The difference comes from the presence or absence of allylic hydrogens. The catalysts were tested for oxidation of propylene.

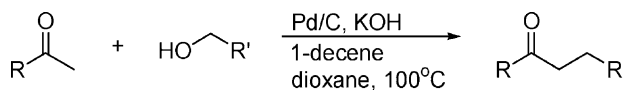


**Chan Sik Cho**

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 55

A palladium-catalyzed route for  $\alpha$ -alkylation of ketones by primary alcohols

A palladium-catalyzed route for  $\alpha$ -alkylation of ketones by primary alcohols ketones are  $\alpha$ -alkylated with primary alcohols in the presence of a catalytic amount of Pd/C and KOH together with 1-decene as sacrificial hydrogen acceptor.

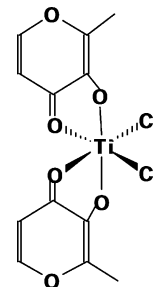


**Paula P. Greco, Rodrigo Brambilla,  
Sandra Einloft, Fernanda C. Stedile,  
Griselda. B. Galland, João H.Z. dos Santos,  
Nara. R. de S. Basso**

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 61

Supported dichlorobis(3-hydroxi-2-methyl-4-pyrone)Ti(IV) catalysts: Evaluation on ethylene polymerization

Titanium complex bearing 3-hydroxi-2-methyl-4-pyrone as ligand was grafted on different inorganic carriers, namely SiO<sub>2</sub>, MAO-modified silica, MCM-41, Al<sub>2</sub>O<sub>3</sub>, ZrO<sub>2</sub> and MgO. The resulting supported catalysts were shown to be active in ethylene polymerization using methylaluminumoxane (MAO) as cocatalyst, most of them being even more active than the homogeneous complex.

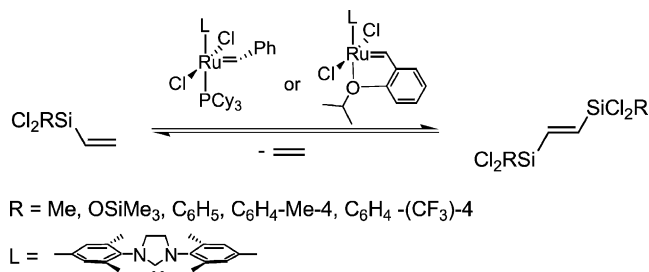


**Cezary Pietraszuk, Bogdan Marciniec,  
Szymon Rogalski, Helmut Fischer**

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 67

Homo-metathesis of vinylsilanes catalysed by ruthenium carbene complexes

The effective homo-metathesis of dichloro-substituted vinylsilanes in the presence of the second generation Grubbs catalyst or the Hoveyda-Grubbs catalyst leads to the selective formation of *E*-1,2-bis(silyl)ethenes and ethene.

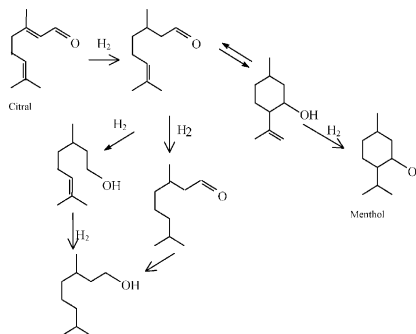


**Päivi Mäki-Arvela, Narendra Kumar, David Kubička, Ali Nasir, Teemu Heikkilä, Vesa-Pekka Lehto, Rainer Sjöholm, Tapio Salmi, Dmitry Yu. Murzin**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 72

One-pot citral transformation to menthol over bifunctional micro- and mesoporous metal modified catalysts: Effect of catalyst support and metal

One-pot liquid phase citral transformation to menthols was conducted over Ni/H-Y and Ni, Ir, Ru, Pd supported on H-MCM-41. The selectivity to menthols decreased in the following order: Ni>Pd>Ru>Ir.

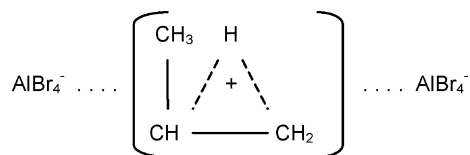


**H.S.A. Douwes**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 82

The kinetics of the aluminium bromide catalyzed isomerization of 1-propyl bromide

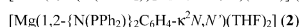
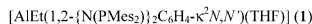
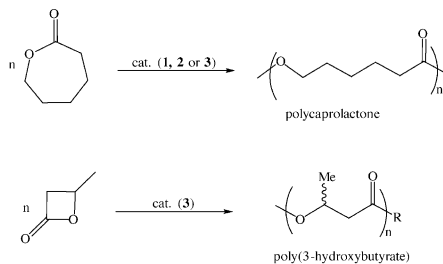
The proposed kinetics of the aluminium bromide catalyzed isomerization of 1-propyl bromide is consistent with a nucleophilic displacement of the aliphatic bromine contained in complexes of the alkyl bromide with aluminium bromide. The displacement, initiated by the  $\text{AlBr}_4^-$  ion, is accompanied by a rate determining 2,1 hydride shift.



**Félicité Majoumo-Mbe, Elena Smolensky, Peter Lönnecke, Dina Shpasser, Moris S. Eisen, Evamarie Hey-Hawkins**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 91

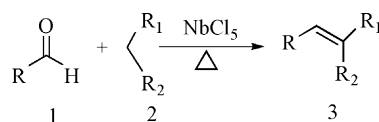
Polymerisations of  $\epsilon$ -caprolactone and  $\beta$ -butyrolactone with Zn-, Al- and Mg-based organometallic complexes



**P. Leelavathi, S. Ramesh Kumar**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 99

Niobium (V) chloride catalyzed Knoevenagel condensation: An efficient protocol for the preparation of electrophilic alkenes

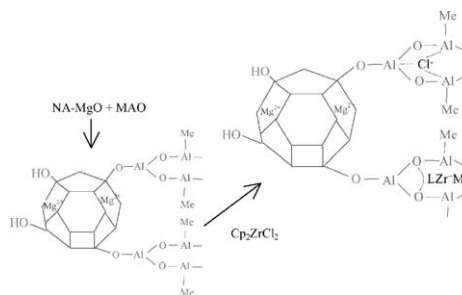


**Mannepalli L. Kantam, Sutapa Ghosh, Khathija Aziz, B. Sreedhar, Boyapati M. Choudary**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 103

Nanoparticle supported bis (cyclopentadienyl) zirconium dichloride catalysts for styrene polymerization

Heterogeneous nanoparticle [NA-MgO/NA-TiO<sub>2</sub>] and MAO supported bis (cyclopentadienyl) zirconium dichloride (Cp<sub>2</sub>ZrCl<sub>2</sub>) catalysts are synthesized and used for the first time for polymerization of styrene monomer to observe how the morphology and the particle shape of the support molecules change the activity of the heterogeneous catalysts for polymerization reactions.

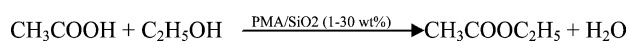


**M.M.M. Abd El-Wahab, A.A. Said**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 109

Phosphomolybdic acid supported on silica gel and promoted with alkali metal ions as catalysts for the esterification of acetic acid by ethanol

Yield of ethyl acetate is effected by catalyst composition, acid–base properties and addition of alkali metal ions.

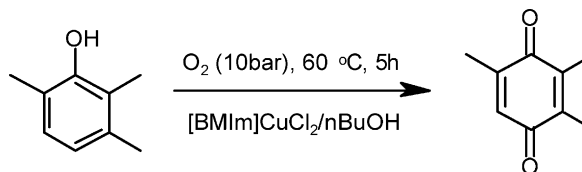


**Hongjian Sun, Xiaoyan Li, Jörg Sundermeyer**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 119

Aerobic oxidation of phenol to quinone with copper chloride as catalyst in ionic liquid

Under different conditions aerobic oxidation of 2,3,6-trimethylphenol to trimethyl-1,4-benzoquinone with copper(II) chloride as catalyst in ionic liquid was studied.

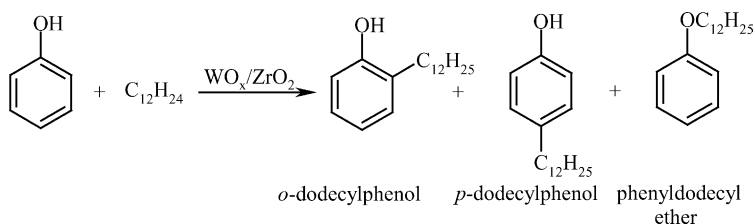


**S. Sarish, Biju M. Devassy, Walter Böhringer, Jack Fletcher, S.B. Halligudi**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 123

Liquid-phase alkylation of phenol with long-chain olefins over WO<sub>x</sub>/ZrO<sub>2</sub> solid acid catalysts

The liquid-phase alkylation of phenol with 1-dodecene was carried out over WO<sub>x</sub>/ZrO<sub>2</sub> solid acid catalysts. The catalyst with 15% WO<sub>3</sub>/ZrO<sub>2</sub> calcined at 800 °C, under the optimized reaction conditions of 120 °C, phenol/1-dodecene molar ratio 2 and time 2 h, gave >99% dodecene conversion with 90% selectivity to dodecylphenol. This catalyst also found to be an efficient catalyst for alkylation of phenol with other long-chain olefins like 1-octene and 1-decene.

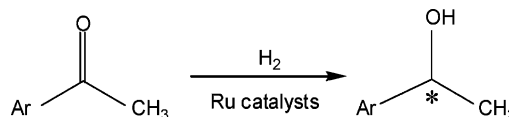


**Yu-Qing Xia, Yuan-You Tang, Zhi-Ming Liang, Chang-Bin Yu, Xiang-Ge Zhou, Rui-Xiang Li, Xian-Jun Li**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 132

Asymmetric hydrogenations of ketones catalyzed by Ru-achiral phosphine-enantiopure diamine complexes

Five new complexes containing achiral phosphines and chiral diamine were synthesized and characterized. Their hydrogenation results indicated that a phosphine ligand which was of a large bite angle or an electron-donated group could improve the catalytic activity in the hydrogenation of carbonyl group. The electron factors of phosphine ligand had no remarkable effects on the e.e. value of hydrogenation products.

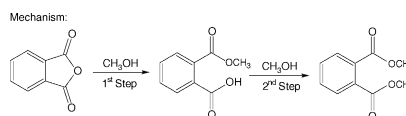


**Seshachalam Udayakumar, Arumugam Pandurangan, Predeep Kumar Sinha**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 139

Mesoporous material as catalyst for the production of fine chemical: Synthesis of dimethyl phthalate assisted by hydrophobic nature MCM-41

Aluminum, iron and zinc containing MCM-41 molecular sieves were prepared by the hydrothermal method. The catalytic activity of these molecular sieves was tested with esterification reaction used with phthalic anhydride (PAH) and methanol (MeOH) in the autoclave at 135, 150 and 175 °C. Conversion increases with increase in temperature, and with an increase in mole ratio. The activity of these catalysts followed the order: Al-MCM-41 (112) > Fe-MCM-41 (115) > Al-MCM-41 (70) > Al-MCM-41 (52) > Fe-MCM-41 (61) > Al, Zn-MCM-41 (104) > Al-MCM-41 (30). The reaction yielded both monomethyl phthalate (MMP) and dimethyl phthalate (DMP). The nature of the catalyst sites has been proposed using water as an impurity. The selectivity of the dimethyl phthalate increases with increase in temperature and increase in mole ratio. The weight of the catalyst was optimized at 0.07g. The hydrophilic and hydrophobic nature of the catalyst has been explained by the influence of water and the external surface acidity also facilitates the reaction and this has been confirmed by the supporting reaction.

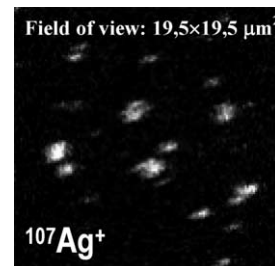


**S. Karski, I. Witońska, J. Rogowski, J. Gólurowska**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 155

Interaction between Pd and Ag on the surface of silica

ToF-SIMS images of the surface of 5% Pd-5% Ag/SiO<sub>2</sub> catalyst show that Ag atoms are not distributed homogeneously but tend to form regions of enhanced Ag concentration. This technique made it possible to observe the changes of catalyst surface which are invisible for XRD.

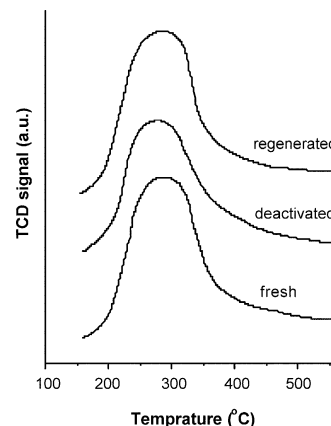


**Dongsen Mao, Guanzhong Lu, Qingling Chen**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 164

Deactivation and regeneration of the B<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub>-ZrO<sub>2</sub> catalyst in the vapor phase Beckmann rearrangement of cyclohexanone oxime

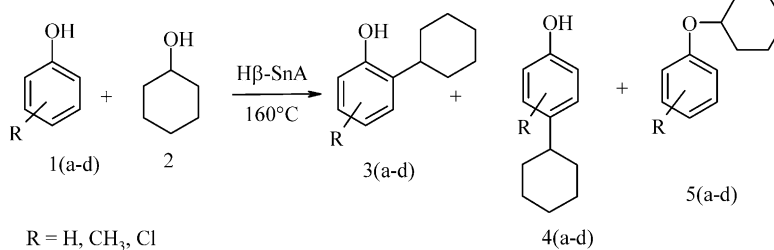
The coke deposition which covers the acid sites is largely responsible for deactivation of the B<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub>-ZrO<sub>2</sub> catalyst. After calcining in air flow at 600 °C for 8 h, the coke deposited on catalyst surface was completely burnt off and the shielded acid sites were again exposed to interact with the reactant molecules and the catalytic activity was fully recovered.



Vivek P. Raje, Ramakrishna P. Bhat,  
Shriniwas D. Samant

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 172

Regioselective *ortho*-C-cyclohexylation of phenols with cyclohexanol in the presence of transition metal modified zeolite-H $\beta$

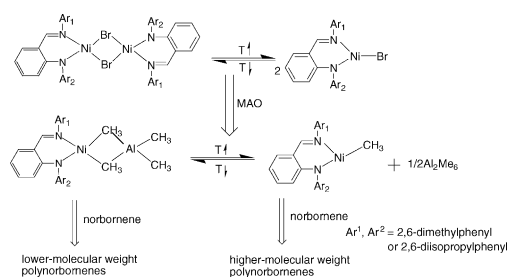


Haiyang Gao, Junkai Zhang, Yan Chen,  
Fangming Zhu, Qing Wu

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 178

Vinyl-polymerization of norbornene with novel anilido-imino nickel complexes/methylaluminoxane: Abnormal influence of polymerization temperature on molecular weight of polynorbornenes

Polynorbornenes obtained by anilido-imino nickel complexes **1–4**/MAO catalytic systems show broad and bimodal molecular weight distribution (MWD) below 50 °C, and average molecular weight of polynorbornenes increases and MWD is narrowed with the increase in the temperature. This abnormal result could be attributed to the equilibrium shift between two active species in toluene.

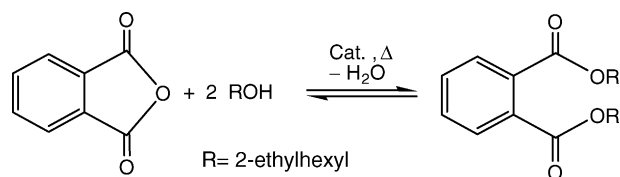


Firdovski Tataroglu Sejidov, Yagoub Mansoori,  
Nadereh Goodarzi

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 186

Esterification reaction using solid heterogeneous acid catalysts under solvent-less condition

The preparation of di-2-ethylhexylphthalate (DOP) via esterification reaction of phthalic anhydride by 2-ethylhexanol in the presence of solid acidic catalysts such as natural and synthetic zeolites, H<sub>4</sub>Si(W<sub>3</sub>O<sub>10</sub>)<sub>4</sub>, and sulfated ZrO<sub>2</sub> has been investigated. Important plasticizers and ester base oils can be prepared from anhydrides/acids and alcohols in the presence of sulfated zirconia under solvent-free condition.



Qi Xie, Luqian Chen, Weizheng Weng,  
Huilin Wan

*Journal of Molecular Catalysis A: Chemical* 240  
(2005) 191

Preparation of MoVTe(Sb)Nb mixed oxide catalysts using a slurry method for selective oxidative dehydrogenation of ethane

Bulk MoVTeNb mixed oxide catalysts, prepared using a traditional slurry method, present highly active and selective for oxidative dehydrogenation of ethane. The orthorhombic M1 phase identified in the catalysts has been shown to be the most active in ethane activation and the most selective for ethene formation.

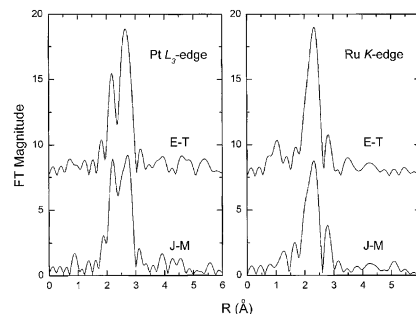


**Din-Goa Liu, Jyh-Fu Lee, Mau-Tsu Tang**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 197

Characterization of Pt-Ru/C catalysts by X-ray absorption spectroscopy and temperature-programmed surface reaction

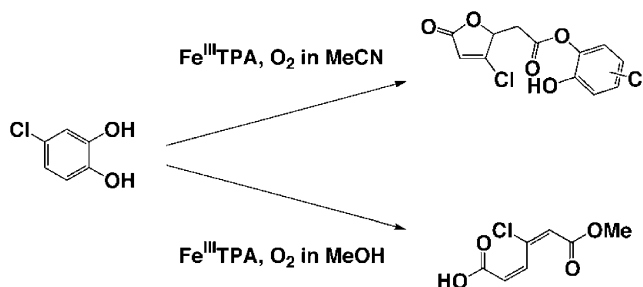
Two commercial Pt-Ru/C catalysts possess bimetallic nanoparticles of similar structure with a Pt-rich core and a Ru-rich shell. However, the percentages of the surface Pt atoms on these two catalysts are slightly different as revealed by X-ray absorption spectroscopy and temperature-programmed surface reaction. Radial distribution functions clearly demonstrate the local atomic structures around Pt and Ru atoms on both samples.

**Yutaka Hitomi, Masakazu Higuchi, Tsunehiro Tanaka, Takuzo Funabiki**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 207

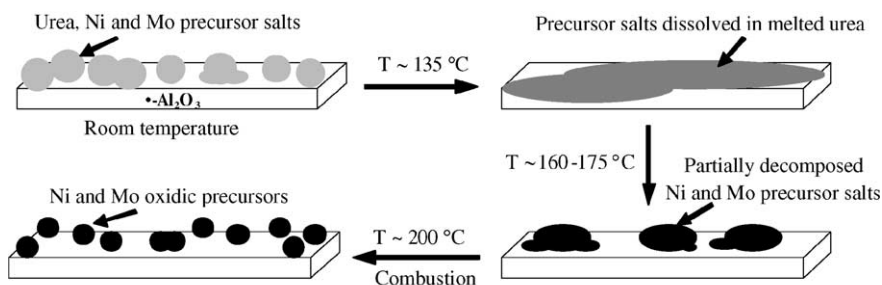
Catalytic oxygenative degradation of 4-chlorocatechol by a nonheme iron(III) complex—Mechanism and prevention of catechol ester formation

The oxygenative degradation of 4-chlorocatechol catalyzed by iron(III)-tris(pyridin-2-yl)amine complex in MeCN gives chlorocatechol esters of the oxygenated products. The efficient catalytic oxygenative degradation of the chlorocatechol is achieved by changing the solvent from MeCN to MeOH, which affords methyl esters of the oxygenated products via efficient methanolysis of muconic anhydride.

**Sergio L. González-Cortés, Tian-Cun Xiao, Serbia M.A. Rodolfo-Baechler, Malcolm L.H. Green**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 214

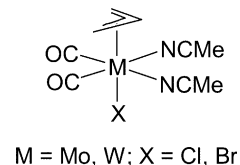
Impact of the urea-matrix combustion method on the HDS performance of Ni-MoS<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> catalysts

**Yoshitaka Yamaguchi, Atsushi Fujita, Noriyuki Suzuki, Takashi Ito**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 226

Metathesis polymerization of norbornene and terminal acetylenes catalyzed by bis(acetonitrile) complexes of molybdenum and tungsten

The ring-opening metathesis polymerization (ROMP) of norbornene catalyzed by bis(acetonitrile) complexes of molybdenum and tungsten, [M(η<sup>3</sup>-C<sub>3</sub>H<sub>5</sub>)Cl(CO)<sub>2</sub>(NCMe)<sub>2</sub>], has been investigated. The poly(norbornene) obtained from this system shows a significantly high *cis* content. These complexes also catalyze the polymerization of terminal acetylenes. A highly active catalytic system for the ROMP of norbornene was achieved by the activation of the tungsten complex with one equivalent of phenylacetylene, and the high *cis* selectivity of the resulting poly(norbornene) was maintained.



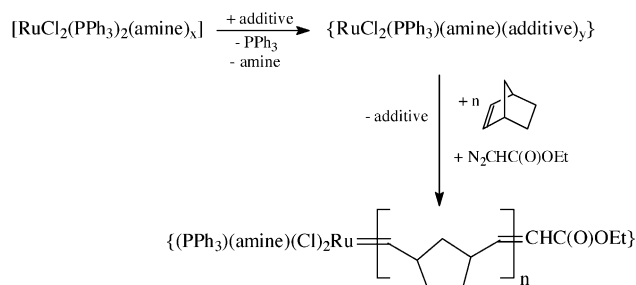


**José Milton E. Matos, Benedito S. Lima-Neto**

*Journal of Molecular Catalysis A: Chemical* 240 (2005) 233

Benefits of donor solvents as additive on ROMP of norbornene catalyzed by amine Ru complexes

The complexes with either piperidine ( $x=1$ ) or imidazole ( $x=2$ ) were tested for ring opening metathesis polymerization of norbornene in the presence of small amounts of common solvents such as additives, with the aim of understanding the influence of these molecules on the catalytic reactivity and on the properties of the resulting polymer.

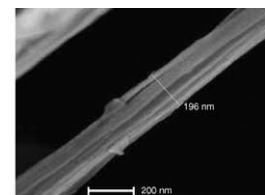


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MCM-41 and SBA-15 supported  $\text{Cp}_2\text{ZrCl}_2$  catalysts for the preparation of nano-polyethylene fibres via in situ ethylene extrusion polymerization

Under atmospheric pressure, nano-polyethylene fibres were prepared via in situ ethylene extrusion polymerization, with MCM-41 and SBA-15 supported zirconocene dichloride ( $\text{Cp}_2\text{ZrCl}_2$ ) catalytic systems, respectively. Experimental results indicate the geometrical structures and surface properties of MCM-41 and SBA-15 have strongly effects on the morphology of the resultant polyethylene, catalytic activity and polymerization rate. Moreover, the resultant polyethylene had higher melting points compared to the homogeneous counterpart.



SEM micrographs of polyethylene fibers prepared by SBA-15-supported catalytic system ([Al]/[Zr]=2000, T=50°C, t=10min)

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Platinum-catalyzed intermolecular hydroamination of terminal alkynes

