

## Contents

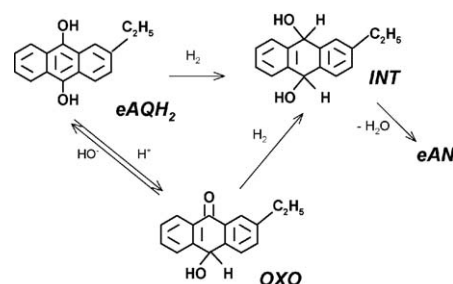
### Articles

**Alicja Drelinkiewicz, Anna Waksmundzka-Góra**

*Journal of Molecular Catalysis A: Chemical 258 (2006) 1*

Hydrogenation of 2-ethyl-9,10-anthraquinone on Pd/SiO<sub>2</sub> catalysts. The role of humidity in the transformation of hydroquinone form

The influence of humidity on the hydrogenation of 2-ethyl-9,10-anthraquinone (eAQ) was studied over 0.5% Pd/SiO<sub>2</sub> catalysts of various Na<sub>2</sub>CO<sub>3</sub> content and thus various alkalinity. Studies are concentrated on the role of water in transformation of eAQH<sub>2</sub>, primary and desirable product which is formed in hydrogenation of eAQ. eAQH<sub>2</sub> can be hydrogenated directly to intermediate product INT or can be tautomerized to OXO isomer with subsequent hydrogenation to INT, the precursor of 2-ethylanthrone (eAN). Humidity facilitates adsorption of reagents in the carbonyl group-bonded configuration thus enhancing the consumption of eAQH<sub>2</sub> by hydrogenolytic reactions and the formation of eAN.

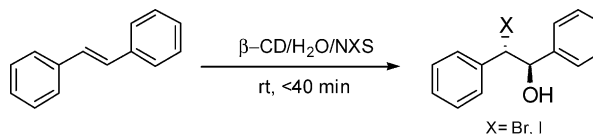


**M. Narender, M. Somi Reddy, Y.V.D. Nageswar, K. Rama Rao**

*Journal of Molecular Catalysis A: Chemical 258 (2006) 10*

Aqueous phase synthesis of *vic*-halohydrins from olefins and *N*-halosuccinimides in the presence of β-cyclodextrin

Various *vic*-halohydrins have been synthesized with *N*-halosuccinimides from olefins in the presence of β-cyclodextrin in water.

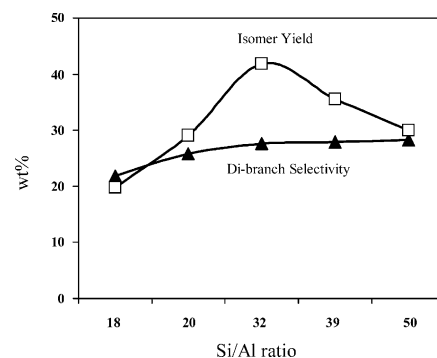


**N. Viswanadham, Lalji Dixit, J.K. Gupta, M.O. Garg**

*Journal of Molecular Catalysis A: Chemical 258 (2006) 15*

Effect of acidity and porosity changes of dealuminated mordenites on *n*-hexane isomerization

The selectivity to di-branched products in *n*-hexane isomerization on mordenites increased with the progress of dealumination. However, the isomer yield reached a maximum upon mild dealumination. The increase in strong acidity and microporosity were responsible for enhanced isomer yields. The selectivity to di-branched products related to the microporosity of the mordenite.

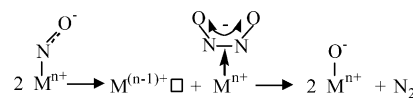


**Runduo Zhang, Adrian Villanueva,  
Houshang Alamdari, Serge Kaliaguine**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 22

Reduction of NO by CO over nanoscale  $\text{LaCo}_{1-x}\text{Cu}_x\text{O}_3$  and  $\text{LaMn}_{1-x}\text{Cu}_x\text{O}_3$  perovskites

Nanoscale  $\text{La}(\text{Co}, \text{Mn})_{1-x}\text{Cu}_x\text{O}_3$  perovskites were generated by reactive grinding. A better catalytic performance in CO + NO reaction was found over  $\text{LaCoO}_3$  compared to  $\text{LaMnO}_3$ , which can be further improved via Cu substitution. This improvement was ascribed to the ease of generation of anion vacancies and the enhancement in lattice oxygen mobility after Cu incorporation. A mechanism was proposed with dissociation of chemisorbed NO forming  $\text{N}_2$  and/or  $\text{N}_2\text{O}$ , and oxidized perovskite surface, with continuous reduction by CO with the production of  $\text{CO}_2$ .

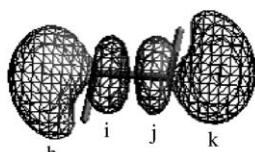


**Hongchang Shi, Yilei Wang, Zhiguo Zhang**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 35

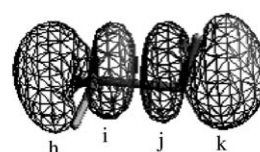
Hydroxylation of alkanes by hydrogen peroxide in superacid: A superelectrophilic active intermediate and an ionization–hydration process

The  $\sigma^*$  orbital energies  $E_{\text{LUMO}\sigma^*}$  of  $\text{HOOH}_2^+$  is 9.39 eV lower than that of neutral  $\text{HOOH}$ . The protonation greatly increase the oxidation activity of hydrogen peroxide.  $\text{HOOH}_2^+$  is an extraordinary superelectrophilic active intermediate of alkane hydroxylation.



$\text{HOOH} \quad E_{\text{LUMO}\sigma^*} = 0.21\text{eV}$

DFT/RB3LYP/6-311G(d,p)



$\text{HOOH}_2^+ \quad E_{\text{LUMO}\sigma^*} = -9.18\text{eV}$

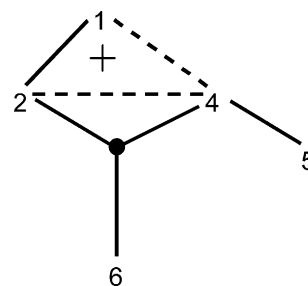
DFT/RB3LYP/6-311G(d,p)

**Ümit Bilge Demirci, François Garin**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 46

A skeletal rearrangement study of a carbon-13 labelled 3-methylpentane on doped sulphated zirconia catalysts

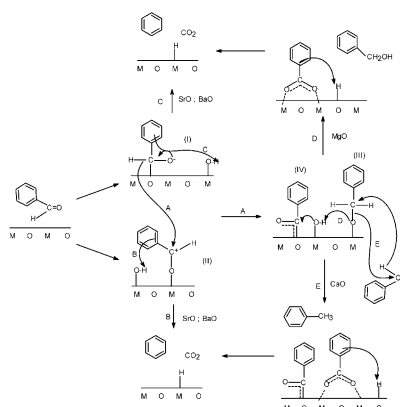
The 3-methyl(3- $^{13}\text{C}$ )pentane isomerization on modified sulphated zirconias could be a one-step reaction, where one or two carbon–carbon bonds could break, involving, e.g. protonated bicyclo-propane as intermediate. The ratio between the proportions of methyl and ethyl migrations could be appreciated as an intrinsic characteristic of the catalyst because of correlations with its physical/chemical characteristics.



**A. Saadi, Z. Rassoul, M.M. Bettahar**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 59

Reduction of benzaldehyde on alkaline earth metal oxides

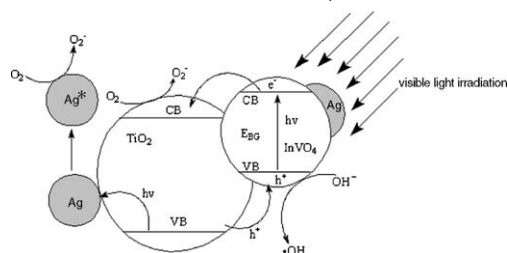


**Lei Ge, Mingxia Xu, Haibo Fang**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 68

Photo-catalytic degradation of methyl orange and formaldehyde by Ag/InVO<sub>4</sub>-TiO<sub>2</sub> thin films under visible-light irradiation

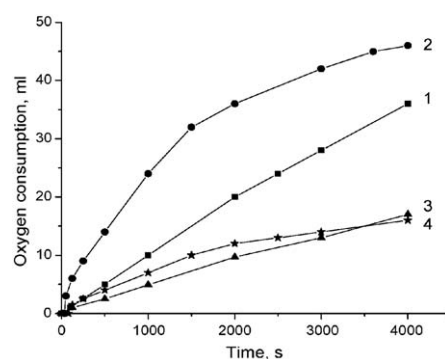
Novel visible-light-activated photo-catalytic Ag/InVO<sub>4</sub>-TiO<sub>2</sub> thin films were prepared through a sol-gel method from the TiO<sub>2</sub> sol containing Ag and InVO<sub>4</sub>. The Ag/InVO<sub>4</sub>-TiO<sub>2</sub> thin films extended the light absorption spectrum toward the visible region; Ag and InVO<sub>4</sub> co-doped thin films significantly enhanced the methyl orange and formaldehyde photo-degradation under visible-light irradiation. The significant enhancement in the Ag/InVO<sub>4</sub>-TiO<sub>2</sub> photo-activity under visible-light irradiation can be ascribed to the simultaneous effects of doped Ag by acting as electron traps and InVO<sub>4</sub> as a narrow band gap sensitizer.

**Yu.M. Sultanov, D. Wöhrle, A.A. Efendiev**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 77

Metal-polymer complex catalysts on the base of polyethyleneimine for oxidation of sulfides

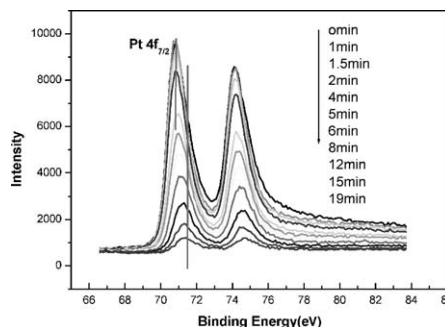
Prearranged polymer metal complexes were prepared on the base of poly(ethyleneimine) and investigated as catalysts in the oxidation of sulfide. The prearranged polymer Cu(II) complexes exhibit catalytic activity comparable with the activity of the commercially employed cobalt(II) phthalocyanine tetrasulfonic acid. Polymer complexes of Ni(II) and Co(II) show a lower catalytic activity. The mechanism of the catalytic oxidation was discussed to explain the different behaviour of the polymer metal complexes.

**Qiuye Li, Ke Wang, Shunli Zhang, Min Zhang, Jianjun Yang, Zhensheng Jin**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 83

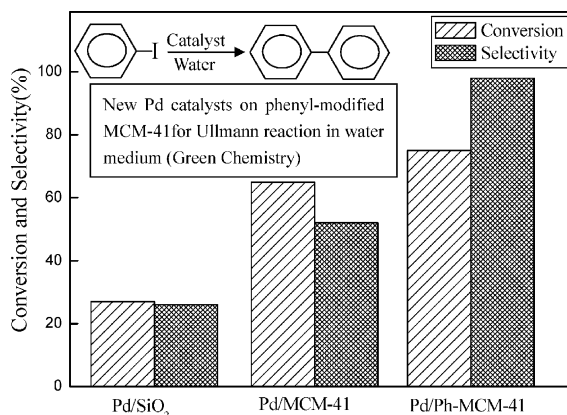
Effect of photocatalytic activity of CO oxidation on Pt/TiO<sub>2</sub> by strong interaction between Pt and TiO<sub>2</sub> under oxidizing atmosphere

The effect of photocatalytic activity of CO oxidation on Pt/TiO<sub>2</sub> catalysts by the strong metal-support interaction (SMSI) between Pt and TiO<sub>2</sub> under oxidizing atmosphere has been investigated. The results show that the SMSI between Pt and TiO<sub>2</sub> occurs when Pt/TiO<sub>2</sub> catalysts are calcined at 673 K in air and the SMSI can improve obviously the photocatalytic activity of CO oxidation.

**Ying Wan, Jia Chen, Dieqing Zhang, Hexing Li**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 89

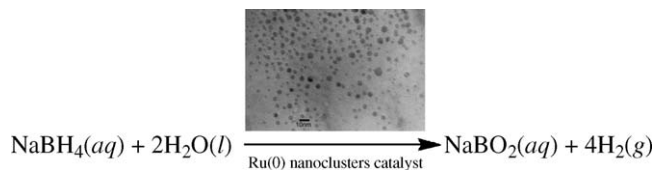
Ullmann coupling reaction in aqueous conditions over the Ph-MCM-41 supported Pd catalyst



**Mehmet Zahmakıran, Saim Özkar**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 95

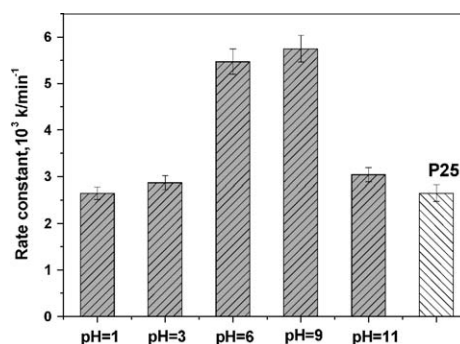
Water dispersible acetate stabilized ruthenium(0) nanoclusters as catalyst for hydrogen generation from the hydrolysis of sodium borohydride

**Jianguo Yu, Yaorong Su, Bei Cheng, Minghua Zhou**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 104

Effects of pH on the microstructures and photocatalytic activity of mesoporous nanocrystalline titania powders prepared via hydrothermal method

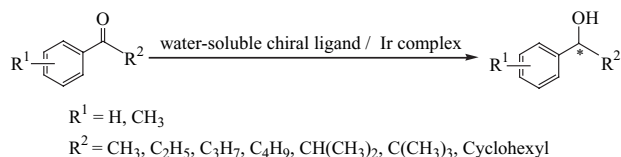
Effects of pH on the microstructures and photocatalytic activity of mesoporous nanocrystalline titania powders prepared via hydrothermal method.

**Bao-Zhu Li, Jian-Shan Chen, Zhen-Rong Dong, Yan-Yun Li, Qing-Biao Li, Jing-Xing Gao**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 113

The novel water-soluble chiral PNNP-type ligand for the enantioselective reduction of ketones in aqueous media

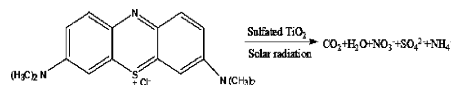
The novel water-soluble chiral Ir-PNNP catalyst serves as an efficient catalyst system for asymmetric transfer hydrogenation of acetophenone derivatives in aqueous media, leading to the corresponding optical alcohols in up to 97% yield and 99% ee.

**P. Mohapatra, K.M. Parida**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 118

Photocatalytic activity of sulfate modified titania 3: Decolorization of methylene blue in aqueous solution

The photocatalytic decolorization of methylene blue was highest under solar radiation compared to adsorption and UV light over sulfate modified titania. The effects of pH, time, adsorbate concentration, catalyst dose,  $\text{H}_2\text{O}_2$ , potassium persulfate and sodium chloride were studied on the percentage of decolorization. While optimising the photocatalytic decolorization conditions it was found that 100 ppm of methylene blue can be completely decolorized using  $1.6 \text{ g L}^{-1}$  of sulfated titania in 4 h under solar radiation.

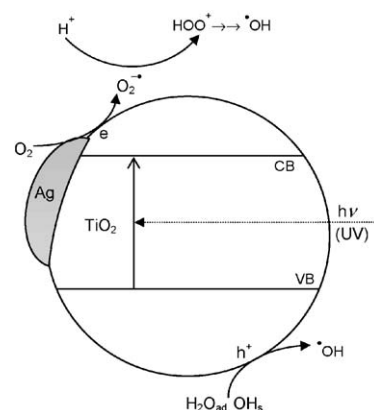


**N. Sobana, M. Muruganadham,  
M. Swaminathan**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 124

Nano-Ag particles doped TiO<sub>2</sub> for efficient photodegradation of Direct azo dyes

Photocatalytic degradation of two Direct diazo dyes, Direct red 23 (DR 23) and Direct blue 53 (DB 53) in the aqueous suspensions of TiO<sub>2</sub> and Ag deposited TiO<sub>2</sub> nanoparticles with UV-A light have been investigated. The enhancement of photocatalytic activity of Ag doped TiO<sub>2</sub> is found to be due to the following mechanism. Ag nanoparticles be deposited on TiO<sub>2</sub> act as electron traps, enhancing the electron-hole separation and the subsequent transfer of the trapped electron to the adsorbed O<sub>2</sub> acting as an electron acceptor.

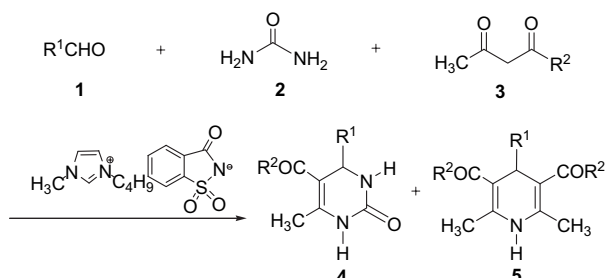


**Ming Li, Wei-Si Guo, Li-Rong Wen,  
Ya-Feng Li, Hua-Zheng Yang**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 133

One-pot synthesis of Biginelli and Hantzsch products catalyzed by non-toxic ionic liquid (BMImSac) and structural determination of two products

Both 1,4-dihydropyridinones (Hantzsch products) and 3,4-dihydropyrimidinones (Biginelli products) were synthesized in one-pot of aldehydes,  $\beta$ -dicarbonyl compounds and urea using non-toxic room temperature ionic liquid 1-*n*-butyl-3-methylimidazolium saccharinate (BMImSac) as catalyst.

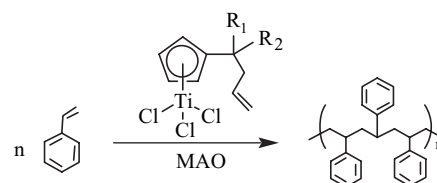


**Chen Wang, Rucheng Liu, Jiling Huang,  
Wei Xiao**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 139

Styrene polymerization with half-sandwich titanium complexes bearing pendent alkenyl groups: From atactic to syndiotactic

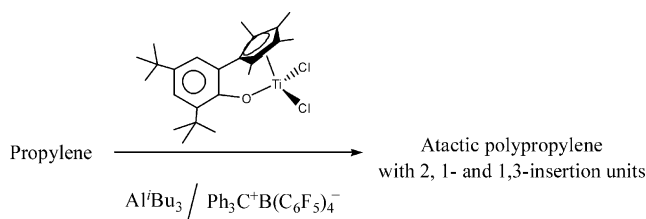
A new series of substituted half-sandwich titanium complexes bearing bridged alkenyl groups [ $\eta^5$ -C<sub>5</sub>H<sub>4</sub>-(bridge)-(alkenyl)]TiCl<sub>3</sub> have been synthesized and characterized. All the titanium complexes display considerable catalytic activity towards the polymerization of styrene in the presence of methylaluminoxane (MAO). Bridging unit between the cyclopentadienyl moiety and the allyl groups plays a crucial role in reactivity and stereoselectivity of styrene polymerisation.



**Chunsheng Lü, Yuetao Zhang, Ying Mu**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 146

Propylene polymerization catalyzed by constrained geometry (cyclopentadienyl)phenoxytitanium catalysts

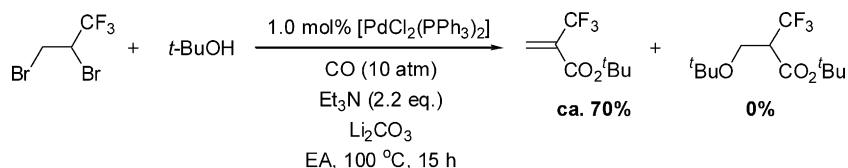


**Yoshikazu Horino, Noriko Wakasa,  
Takamasa Fuchikami, Tetsu Yamakawa**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 152

An industrially usable Pd-catalyzed carboalkoxylation of 1,2-dibromo-3,3,3-trifluoropropane to *tert*-butyl trifluoromethacrylate in the presence of an inorganic base

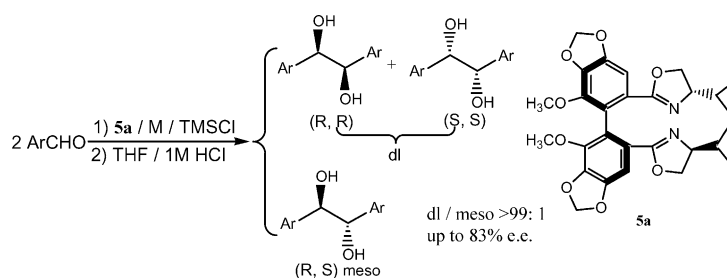
Pd-catalyzed carboalkoxylation of 1,2-dibromo-3,3,3-trifluoropropane with *tert*-butyl alcohol to provide *tert*-butyl trifluoromethacrylate was improved from a practical standpoint. The addition of an inorganic base, specifically  $\text{Li}_2\text{CO}_3$ , surmounted the previous disadvantages of low reactivity and selectivity.  $\text{Li}_2\text{CO}_3$  not only accelerated the reaction drastically but also suppressed the further reaction of the methacrylate and alcohol completely.



**Jiwu Wen, Qitao Tan, Tianpa You**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 159

Biphenyl-oxazoline ligands derived from  $\beta$ -DDB: Their synthesis and application in asymmetric pinacol coupling reaction

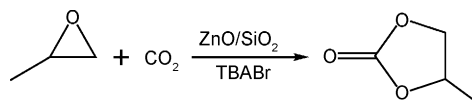


**Michael Ramin, Niels van Vegten,  
Jan-Dierk Grunwaldt, Alfons Baiker**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 165

Simple preparation routes towards novel Zn-based catalysts for the solventless synthesis of propylene carbonate using dense carbon dioxide

Differently prepared supported and unsupported zinc-based catalysts were tested in the solventless synthesis of propylene carbonate.  $\text{ZnO-SiO}_2$  xerogels prepared by the sol-gel method and flame-made  $\text{ZnO-SiO}_2$  materials synthesized by flame spray pyrolysis exhibited a good catalytic activity. A significant improvement of the flame-made  $\text{ZnO-SiO}_2$  catalysts could be achieved by depositing the zinc precursor on pre-formed silica particles. Not single site zinc but rather zinc-clusters play an important role in the catalytic activity of the system, as also evidenced by EXAFS results and SEM.

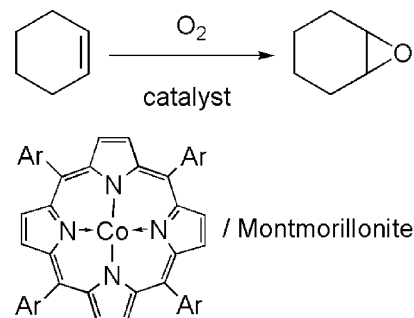


**Hideyuki Kameyama, Fumitaka Narumi,  
Tetsutaro Hattori, Hiroshi Kameyama**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 172

Oxidation of cyclohexene with molecular oxygen catalyzed by cobalt porphyrin complexes immobilized on montmorillonite

Composite materials were prepared by intercalating cationic porphyrinato cobalt complexes into a montmorillonite interlayer. The catalytic activity of these composite materials was remarkably high in the oxidation of cyclohexene by oxygen molecules in the presence of isobutyraldehyde, compared with the homogeneous complex catalyst. Especially, the tetrakis(1-ethyl-3-pyridinio)porphyrinato cobalt complex fixed between montmorillonite layers showed the highest catalytic activity.

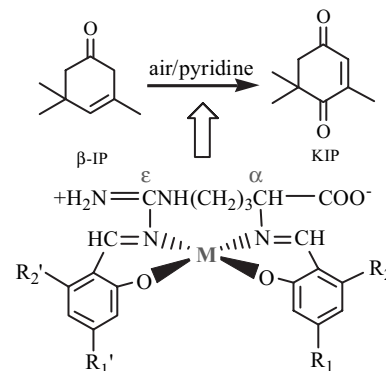


**Jiayong Mao, Ning Li, Haoran Li,  
Xingbang Hu**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 178

Novel Schiff base complexes as catalysts in aerobic selective oxidation of  $\beta$ -isophorone

A series of novel Schiff base complexes were synthesized on the bases of arginine, which has two kinds of asymmetric  $-\text{NH}_2$ . The asymmetric complexes have been proven to be an efficient catalyst with high activity and selectivity in the oxidation of  $\beta$ -isophorone to keto-isophorone.

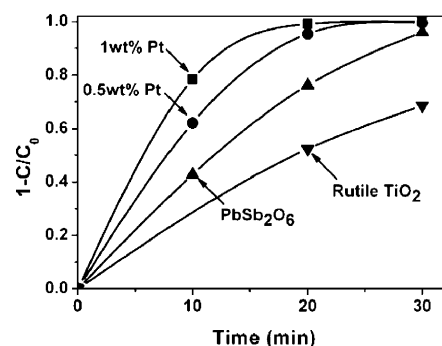


**Ke-Lei Zhang, Xin-Ping Lin, Fu-Qiang Huang,  
Wen-Deng Wang**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 185

A novel photocatalyst  $\text{PbSb}_2\text{O}_6$  for degradation of methylene blue

$\text{PbSb}_2\text{O}_6$  is more active in photodegrading MB than rutile  $\text{TiO}_2$  under UV light illumination. The 1 wt.% Pt dispersion on  $\text{PbSb}_2\text{O}_6$  powder surface doubles the photocatalytic efficiency.

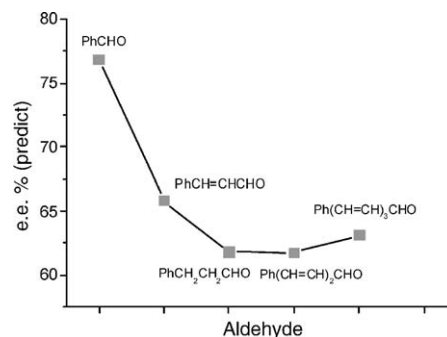


**Jiang Chen, Wen Jiwu, Li Mingzong,  
Tianpa You**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 191

Calculation on enantiomeric excess of catalytic asymmetric reactions of diethylzinc addition to aldehydes with topological indices and artificial neural network

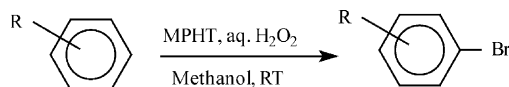
The relationships between the enantiomeric excess of products and the structures of the catalysts or reagents in several types of asymmetric diethylzinc addition reactions were studied by using the BP neural network with topological indices. Moderate cross-validated correlation coefficients were yielded by the models generated from the neural network. Then the models were further used to validate reaction mechanisms, determine the proper reaction environment, and predict the activities of new catalysts.



**Sweety Singhal, Suman L. Jain, Bir Sain**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 198

A simple and improved regioselective bromination of aromatic compounds using *N*-methylpyrrolidin-2-one hydrotribromide and aqueous hydrogen peroxide under mild reaction conditions

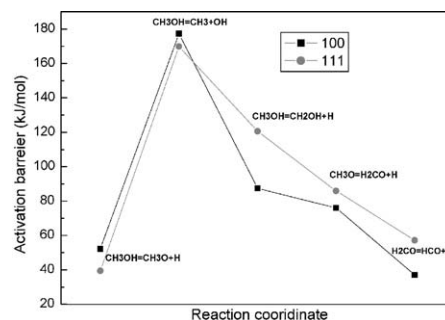


**Yu-Hua Zhou, Pei-Hong Lv, Gui-Chang Wang**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 203

DFT studies of methanol decomposition on Ni(1 0 0) surface: Compared with Ni(1 1 1) surface

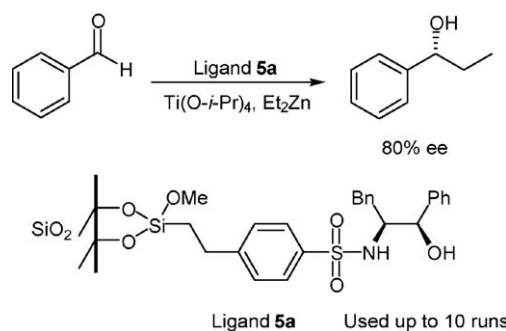
Both of the C–H bond and O–H bond broken are the favorable reaction paths on Ni(1 0 0), which is different from the case of Ni(1 1 1) in which only the O–H bond broken is the preferred reaction path.

**Lu-Ning Huang, Xin-Ping Hui, Peng-Fei Xu**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 216

Asymmetric addition of diethylzinc to benzaldehyde catalyzed by silica-immobilized titanium(IV) complexes of *N*-sulfonylated amino alcohols

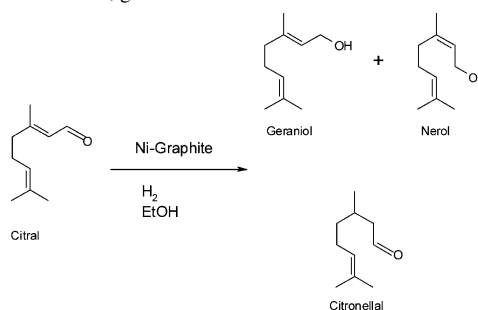
Silica-immobilized titanium(IV) complexes of sulfonylated amino alcohols were used for the asymmetric addition of diethylzinc to benzaldehyde with good enantioselectivity (80% e.e.). The catalyst was able to be recovered and reused in multiple catalytic runs (up to 10 times) without loss of enantioselectivity.

**M. Cerro-Alarcón, B. Bachiller-Baeza, A. Guerrero-Ruiz, I. Rodríguez-Ramos**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 221

Effect of the reduction–preparation method on the surface states and catalytic properties of supported-nickel particles

Only Ni<sup>0</sup> sites were detected at the surface of the Ni/graphite catalysts prepared by reduction with hydrogen leading to high selectivity towards citronellal formation, while Ni oxidised species are also present (and are major) for catalysts prepared by reduction with hydrazine, what leads to an enhanced selectivity towards the formation of the unsaturated alcohols, geraniol and nerol.

**Ned A. Stephenson, Alexis T. Bell**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 231

The influence of substrate composition on the kinetics of olefin epoxidation by hydrogen peroxide catalyzed by iron(III) [tetrakis(pentafluorophenyl)] porphyrin

UV–visible and NMR spectroscopies indicate that norbornene and cyclohexene coordinate axially to iron(III) [tetrakis(pentafluorophenyl)] porphyrin, while cyclooctene, *cis*-stilbene, and styrene do not. The observed reaction rate and final yield for the iron(III) [tetrakis(pentafluorophenyl)] porphyrin chloride catalyzed epoxidation of olefins by H<sub>2</sub>O<sub>2</sub> is independent of the substrate if the substrate does not coordinate to the iron center of the porphyrin.

Substrate	k <sub>obs</sub> (min <sup>-1</sup> )	Yield
cyclooctene	0.25 ± 0.02	88 ± 2%
<i>cis</i> -stilbene <sup>a</sup>	0.26 ± 0.04	88 ± 4%
styrene	0.26 ± 0.03	88 ± 2%
norbornene <sup>b</sup>	0.07 ± 0.01	45 ± 2%
cyclohexene <sup>c</sup>	0.18 ± 0.04	74 ± 3%

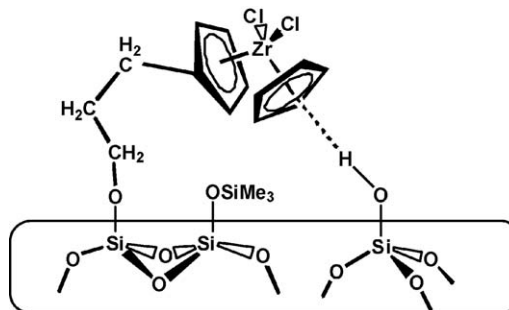


**Pedro Carrión, Fernando Carrillo-Hermosilla, Carlos Alonso-Moreno, Antonio Otero, Antonio Antiñolo, José Sancho, Elena Villaseñor**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 236

Supported modified zirconocene catalyst for ethylene polymerization

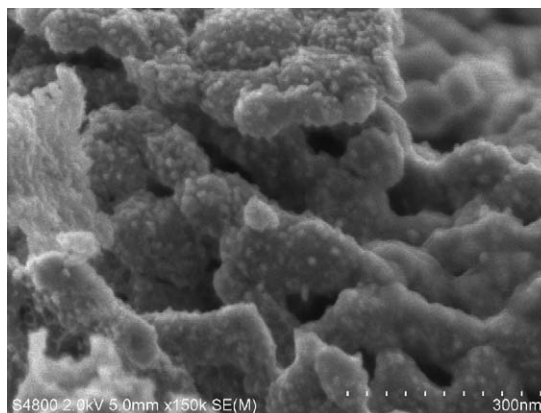
The reactivity of the silyl ether-substituted zirconocene  $[\text{Zr}\{\eta^5\text{-C}_5\text{H}_4(\text{CH}_2)_3\text{OSiMe}_3\}(\eta^5\text{-C}_5\text{H}_5)\text{Cl}_2]$  towards different supports based on dehydroxylated silica was evaluated and comparative studies with respect to the unmodified analogue  $[\text{Zr}(\eta^5\text{-C}_5\text{H}_5)_2\text{Cl}_2]$  were performed.



**Markus J. Koponen, Tapani Venäläinen, Mika Suvanto, Kauko Kallinen, Toni-J.J. Kinnunen, Matti Härkönen, Tapani A. Pakkanen**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 246

Methane conversion and  $\text{SO}_2$  resistance of  $\text{LaMn}_{1-x}\text{Fe}_x\text{O}_3$  ( $x = 0.4, 0.5, 0.6, 1$ ) perovskite catalysts promoted with palladium

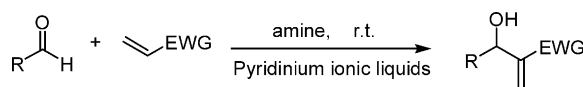


**San-Hu Zhao, Hai-Rong Zhang, Li-Heng Feng, Zhao-Bin Chen**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 251

Pyridinium ionic liquids-accelerated amine-catalyzed Morita–Baylis–Hillman reaction

Several ionic liquids were used for Morita–Baylis–Hillman reaction; the results show that the pyridinium ionic liquids *N*-ethylpyridinium tetrafluoroborate ( $[\text{EPy}][\text{BF}_4]$ ) and *N*-butylpyridinium nitrate ( $[\text{BuPy}][\text{NO}_3]$ ) as reaction media were efficient for DABCO-catalyzed Morita–Baylis–Hillman reaction. In short reaction time, good yields have been obtained. In addition, in the presence of ionic liquid  $[\text{EPy}][\text{BF}_4]$ , the hexamethylenetetramine (HMTA), a cheap tertiary amine, effectively catalyzed the Morita–Baylis–Hillman reaction.



R = Aryl, Alkyl; EWG = CN,  $\text{COOCH}_3$

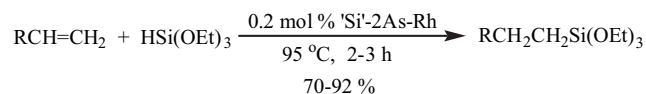
Pyridinium ionic liquids :  $[\text{EPy}][\text{BF}_4]$ ,  $[\text{BuPy}][\text{NO}_3]$

**Gang Liu, Mingzhong Cai**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 257

Synthesis of a novel fumed silica-supported bidentate arsine rhodium complex and its catalytic behavior in the hydrosilylation of olefins with triethoxysilane

A novel fumed silica-supported poly-4-oxa-6,7-bis(diphenylarsino)heptylsiloxane rhodium complex was prepared by treatment of poly-4-oxa-6,7-dichloroheptylsiloxane with potassium diphenylarsenide in THF and then reaction with rhodium chloride. It was found that this complex is an efficient catalyst for hydrosilylation of a variety of olefins with triethoxysilane.

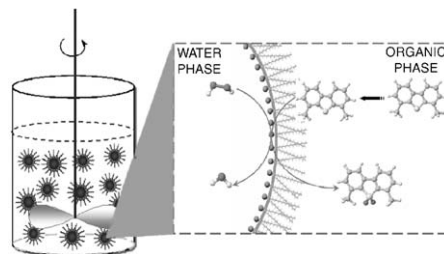


**Jinbo Gao, Shouguo Wang, Zongxuan Jiang,  
Hongying Lu, Yongxing Yang, Fei Jing, Can Li**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 261

Deep desulfurization from fuel oil via selective oxidation using an amphiphilic peroxotungsten catalyst assembled in emulsion droplets

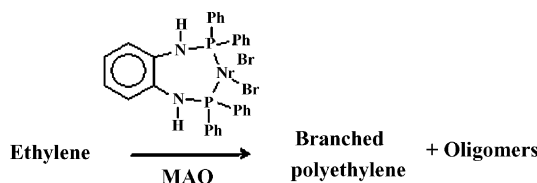
A recyclable amphiphilic catalyst assembled in the interface of the emulsion droplets, shows high selectivity and activity in the oxidation of sulfur-containing molecules to sulfones with hydrogen peroxide in diesel under mild reaction conditions. The emulsion catalytic systems are not only in the highly dispersed form but also behave like homogenous catalyst with high activity. All the sulfur-containing molecules present in diesel can be completely oxidized into sulfones with ~100% selectivity of sulfones in W/O (H<sub>2</sub>O<sub>2</sub>-in-diesel) emulsion system. The sulfones can be readily separated from the diesel, and the sulfur level of the desulfurized diesel can be lowered from about 500 ppm to below 1 ppm with about 98% yield of oil.



**Mauro C.B. Dolinsky, Whei O. Lin,  
Marcos L. Dias**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 267

Ethylene polymerization with nickel complexes containing aminophosphine ligands



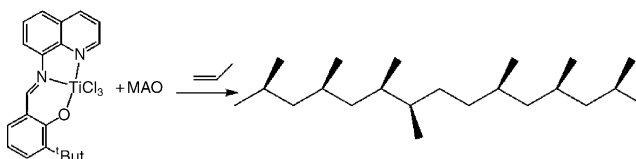
**Gino Paolucci, Alessandra Zanella,  
Laura Sperti, Valerio Bertolasi, Mina Mazzeo,  
Claudio Pellecchia**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 275

Tridentate [N,N,O] Schiff-base group 4 metal complexes: Synthesis, structural characterization and reactivity in olefin polymerization

The three completely characterized octahedral complexes, LTiCl<sub>3</sub>(1), LZrCl<sub>3</sub>(2) and LHfCl<sub>3</sub>(3) (L = (*E*)-2-*tert*-butyl-6[(quinoline-8-ylimino)methyl]phenolate) were tested as catalysts for ethylene and propylene polymerization under a variety of experimental conditions. Titanium complex 1, activated by MAO afforded, at low temperature, an isotactic polypropylene ([mm] = 80%) containing 5% isolated regioirregular units in *threo* configuration.

The analysis of the stereoerrors present in the methyl region of its <sup>13</sup>C NMR spectrum are consistent with an "enantiomorphic site" mechanism of steric control and suggest that both primary and secondary monomer insertions occur with the same enantioface selectivity.

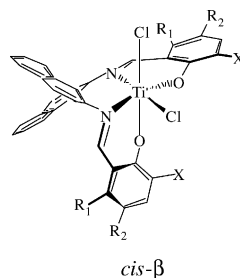


**Maria Strianese, Marina Lamberti,  
Mina Mazzeo, Consiglia Tedesco,  
Claudio Pellecchia**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 284

Polymerization of ethylene and propene promoted by binaphthyl-bridged Schiff base complexes of titanium

Three new binaphthyl-bridged Schiff base complexes featuring different phenolate substituents (*meta*-Me, *ortho,para*-di-Cl, *ortho,para*-di-Br) were synthesized. NMR analysis indicated that the *cis*-β isomers are preferentially formed in any case. These complexes were tested as precatalysts for ethylene and propene polymerization comparing their behaviour to that of related titanium and zirconium complexes previously reported.



L<sup>2</sup>TiCl<sub>2</sub>: R<sub>1</sub> = Me, R<sub>2</sub> = H, X = *t*-Bu

L<sup>3</sup>TiCl<sub>2</sub>: R<sub>1</sub> = H, R<sub>2</sub> = X = Cl

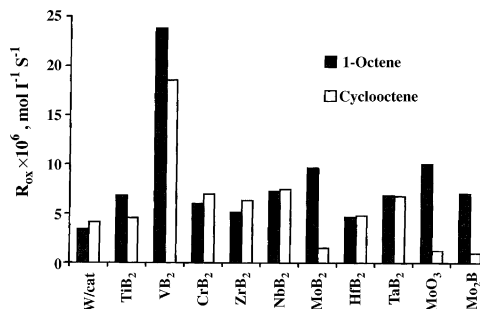
L<sup>4</sup>TiCl<sub>2</sub>: R<sub>1</sub> = H, R<sub>2</sub> = X = Br

**Yu. Trach, B. Schulze, O. Makota, L. Bulgakova**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 292

The liquid-phase oxidation of olefins by molecular oxygen in the presence of metal borides and MoO<sub>3</sub>

The results of investigation of initial stages of the liquid-phase oxidation of 1-octene and cyclooctene by molecular oxygen in the presence of transition metal borides and MoO<sub>3</sub> are reported. The oxidation process of 1-octene is activated by molybdenum compounds whereas the oxidation of cyclooctene is inhibited by them.

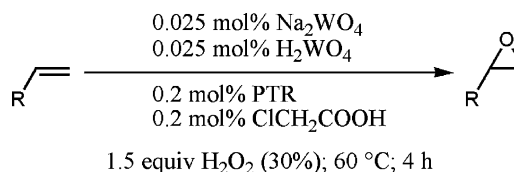


**Palanisamy Uma Maheswari, Xiaohua Tang, Ronald Hage, Patrick Gamez, Jan Reedijk**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 295

The role of carboxylic acids on a Na<sub>2</sub>WO<sub>4</sub>/H<sub>2</sub>WO<sub>4</sub>-based biphasic homogeneous alkene epoxidation, using H<sub>2</sub>O<sub>2</sub> as oxidant

Screening of various carboxylic acids as acid additives with different substituents with the catalyst system below towards alkene epoxidation, leads to the observation that the substituted/unsubstituted acetic and benzoic acids generally enhance the rate of the epoxidation while salicylic acids significantly decrease the catalyst activity and chloroacetic acid as the best additive to enhance the rate of epoxidation.

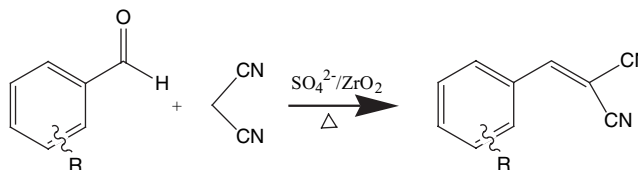


**Benjaram M. Reddy, Meghshyam K. Patil, Komateedi N. Rao, Gunugunuri K. Reddy**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 302

An easy-to-use heterogeneous promoted zirconia catalyst for Knoevenagel condensation in liquid phase under solvent-free conditions

The sulfate-ion promoted ZrO<sub>2</sub> has been employed for Knoevenagel condensation of various aliphatic, aromatic and heterocyclic aldehydes with malononitrile in one step. This catalyst facilitates the reaction under solvent-free conditions and provides good product yields.

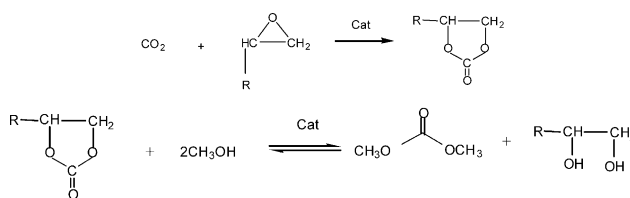


**Hui Wang, Mouhua Wang, Shuigang Liu, Ning Zhao, Wei Wei, Yuhan Sun**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 308

Influence of preparation methods on the structure and performance of CaO-ZrO<sub>2</sub> catalyst for the synthesis of dimethyl carbonate via transesterification

The activity and stability of CaO-ZrO<sub>2</sub> catalysts for the synthesis of dimethyl carbonate via transesterification (Scheme 1) was greatly influenced by the preparation method and calcination temperature. It was found that the homogeneous CaO-ZrO<sub>2</sub> solid solution exhibited both excellent activity and stability because of the strong interaction between active sites and support.



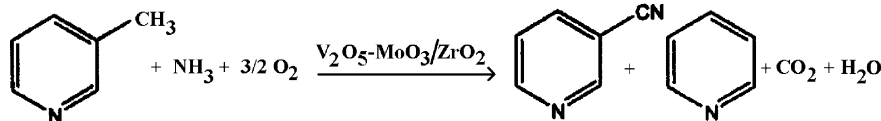
Scheme 1 Synthesis of DMC by transesterification

**Komandur V.R. Chary,  
Chinthala Praveen Kumar, Taduri Rajiah,  
Chakravartula S. Srikanth**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 313

Dispersion and reactivity of monolayer vanadium oxide catalysts supported on zirconia: The influence of molybdena addition

ZrO<sub>2</sub> is an interesting support to investigate the dispersion of vanadia and catalytic properties of V<sub>2</sub>O<sub>5</sub>-MoO<sub>3</sub> catalysts. This paper provides influence of MoO<sub>3</sub> on the dispersion and catalytic properties of vanadium oxide supported on ZrO<sub>2</sub>. These catalysts are found to be highly active and selective for the vapour phase ammoxidation of 3-picoline to nicotinonitrile.



**Praveen K. Tandon, Sumita Sahgal,  
Alok K. Singh, Santosh Kumar, Mamta Dhusia**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 320

Oxidation of cyclic ketones by cerium(IV) in presence of iridium(III) chloride

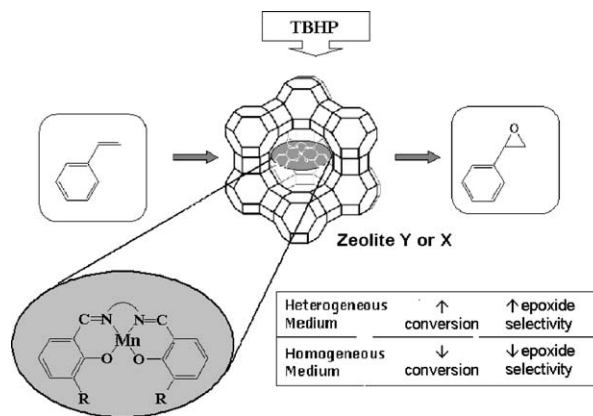
IrCl<sub>3</sub> in acidic medium was found more effective catalyst than RuCl<sub>3</sub> or OsO<sub>4</sub> in the oxidation of cyclic ketones by ceric perchlorate. Conversion of hydrolyzed to un-hydrolyzed species of cerium with increasing acid concentrations, its reduction by water and spectral evidence for 2-hydroxy ketone as intermediate in the oxidation was verified.

$$-d[\text{Ce}^{\text{IV}}]/dt = \frac{2 k K_1 K_2 [\text{Ce}^{\text{IV}}][\text{S}][\text{Ir}^{\text{III}}][\text{H}^+]}{1 + K_1 K_2 [\text{Ce}^{\text{IV}}][\text{S}]}$$

**M. Silva, C. Freire, B. de Castro,  
J.L. Figueiredo**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 327

Styrene oxidation by manganese Schiff base complexes in zeolite structures

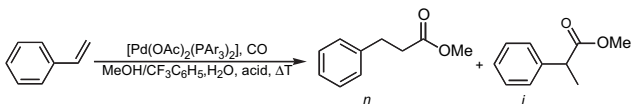


**Jeroen J.M. de Pater, Berth-Jan Deelman,  
Cornelis J. Elsevier, Gerard van Koten**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 334

Lightly fluororous [Pd(OAc)<sub>2</sub>{P(C<sub>6</sub>H<sub>4</sub>-*p*-SiMe<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>C<sub>6</sub>F<sub>13</sub>)<sub>3</sub>}]<sub>2</sub> in the methoxycarbonylation of styrene: Formation, performance and stability of the catalyst system

The fluororous complex [Pd(OAc)<sub>2</sub>{P(C<sub>6</sub>H<sub>4</sub>-*p*-SiMe<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>C<sub>6</sub>F<sub>13</sub>)<sub>3</sub>}]<sub>2</sub> was applied in the methoxycarbonylation of styrene. Significant differences in activity, selectivity and stability compared to its non-fluorous analogue were observed. The results are relevant for the development of a fluororous biphasic approach to the recycling of Pd-based alkoxy carbonylation catalysts.

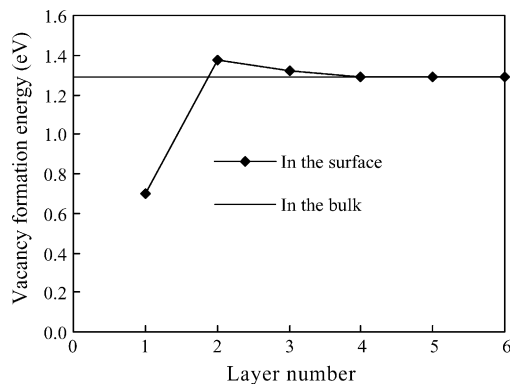


[Pd(OAc)<sub>2</sub>(PAr<sub>3</sub>)<sub>2</sub>] = [Pd(OAc)<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>] (1) or [Pd(OAc)<sub>2</sub>(P(C<sub>6</sub>H<sub>4</sub>-*p*-SiMe<sub>2</sub>(CH<sub>2</sub>CH<sub>2</sub>C<sub>6</sub>F<sub>13</sub>)))<sub>2</sub>] (2)

**Guo-Xiang Chen, Jian-Min Zhang, Ke-Wei Xu, Vincent Ji**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 341

Computer simulation study of self-diffusion in Pd(111) surface

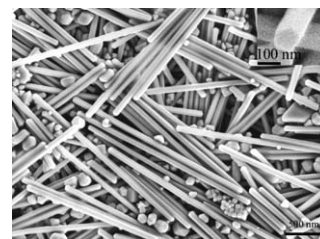


**R.J. Chimentão, F. Medina, J.L.G. Fierro, J.E. Sueiras, Y. Cesteros, P. Salagre**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 346

Styrene epoxidation over cesium promoted silver nanowires catalysts

Epoxidation of styrene to styrene oxide by molecular oxygen was studied over cesium promoted silver nanowires catalysts. The catalytic activity shows a maximum for silver nanowires promoted with 0.25 wt.% of Cs, achieving 94.6% of conversion and total selectivity to desired oxidation products (styrene oxide and phenylacetaldehyde). Negligible deactivation of the catalyst was observed over 30 days of reaction.

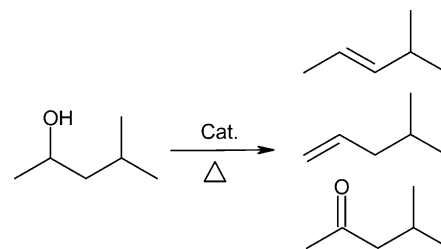


**Benjaram M. Reddy, Pandian Lakshmanan, Pankaj Bharali, Pranjal Saikia**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 355

Dehydration of 4-methylpentan-2-ol over  $Ce_xZr_{1-x}O_2/SiO_2$  nano-composite catalyst

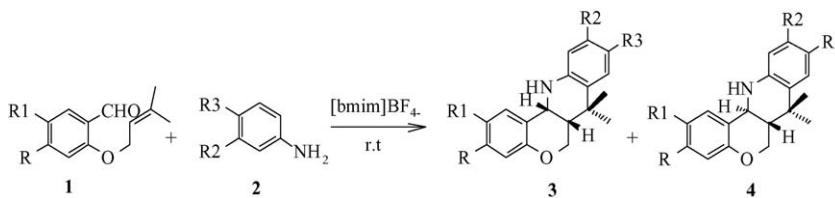
The nano-sized  $Ce_xZr_{1-x}O_2$  solid solution over silica support exhibits stable catalytic activity for the dehydration of 4-methylpentan-2-ol to 4-methylpent-1-ene in vapour phase under normal atmospheric pressure. The thermal and textural stability of the catalyst was investigated by means of XRD, HREM, XPS and BET surface area methods to correlate with the catalytic properties.



**J.S. Yadav, B.V. Subba Reddy, G. Kondaji, S. Sowjanya, K. Nagaiah**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 361

Intramolecular imino-Diels-Alder reactions in [bmim]BF<sub>4</sub> ionic medium: Green protocol for the synthesis of tetrahydrochromanoquinolines

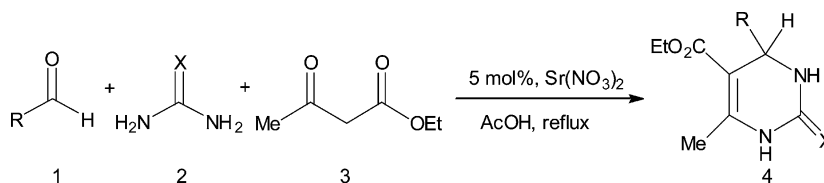


**Chenjiang Liu, Jide Wang, Yanping Li**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 367

One-pot synthesis of 3,4-dihydropyrimidin-2(1H)-thiones using strontium(II) nitrate as a catalyst

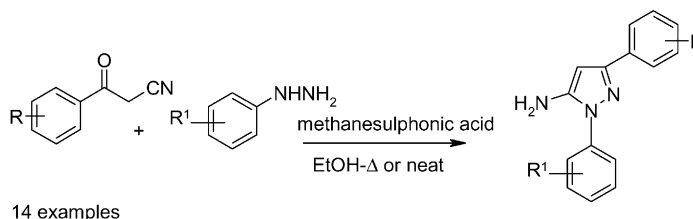
A simple, efficient method for the one-pot Biginelli condensation reaction of aldehydes, ethyl acetoacetate and urea or thiourea employing strontium(II) nitrate as a novel catalyst is described in good yields. The catalyst exhibited remarkable reactivity.



**N. Suryakiran, T. Srikanth Reddy,  
K. Asha Latha, P. Prabhakar, K. Yadagiri,  
Y. Venkateswarlu**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 371

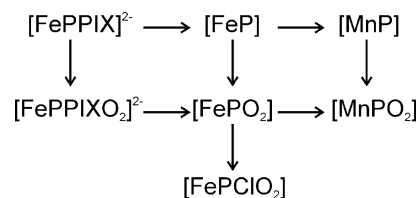
An expeditious synthesis of 3-amino 2H-pyrazoles promoted by methanesulphonic acid under solvent and solvent free conditions

**Dorota Rutkowska-Zbik, Malgorzata Witko**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 376

Following nature—Theoretical studies on factors modulating catalytic activity of porphyrins

The present paper aims to study how modifications in the porphyrin complexes may change their catalytic properties. The investigated parameters comprise change of the central metal ion and porphyrin substituents. The obtained theoretical results are discussed in terms of dioxygen-binding energies, bond lengths, bond orders as well as charges on the selected fragments of the studied catalysts.

**K.M. Parida, Dharitri Rath**

*Journal of Molecular Catalysis A: Chemical* 258 (2006) 381

Studies on MCM-41: Effect of sulfate on nitration of phenol

S/MCM-41 is an efficient catalyst for nitration of phenol, which is an electrophilic substitution reaction. The electrophile, i.e. nitronium ion was generated by the reaction between HNO<sub>3</sub> and the Brønsted acid sites of S/MCM-41. It attacked phenol and gave *ortho*- and *para*-nitrophenol. Between these two products *ortho*-nitrophenol was the major product.

