

## Contents

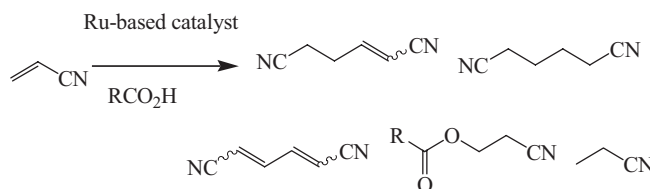
### Articles

**Kohich Kashiwagi, Ryoji Sugise,  
Toshihiro Shimakawa, Tunao Matuura,  
Masashi Shirai**

*Journal of Molecular Catalysis A: Chemical 264  
(2007) 9*

Ruthenium-catalyzed dimerization of acrylonitrile  
in the presence of carboxylic acids

The catalyst system using the combination of ruthenium-based catalyst and carboxylic acid is useful for the tail-to-tail dimerization of acrylonitrile without the formation of undesired by-product propionitrile. Carboxylic acids having  $pK_a$  1.8–5.0 are suitable as co-catalyst for the dimerization of acrylonitrile. Carboxylic acids are considered to be effective in the protonolysis step of the carbon–ruthenium bond of intermediate Ru complex.

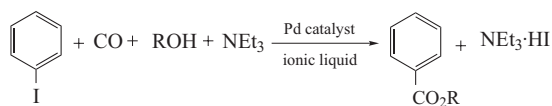


**Qi Lin, Chaofen Yang, Weidong Jiang,  
Hua Chen, Xianjun Li**

*Journal of Molecular Catalysis A: Chemical 264  
(2007) 17*

Carbonylation of iodobenzene catalyzed by water-  
soluble palladium–phosphine complexes in ionic  
liquid

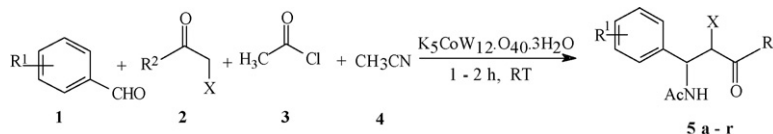
The carbonylation of iodobenzene catalyzed by water-soluble palladium–TPPTS complex has been investigated in ionic liquid [bmim][*p*-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>]. The combination of palladium–TPPTS complex and [bmim][*p*-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>] exhibits excellent catalytic activity and selectivity. The catalyst can be reused for 10 times.



**Lingaiah Nagarapu, Srinivas Kantevari,  
Venkata Narasimhaji Cheemalapati,  
Satyender Apuri, N. Vijaya Kumari**

*Journal of Molecular Catalysis A: Chemical 264  
(2007) 22*

Potassium dodecatungstocobaltate trihydrate  
(K<sub>5</sub>CoW<sub>12</sub>O<sub>40</sub>·3H<sub>2</sub>O): A mild and efficient reusable  
catalyst for the synthesis of β-acetamido ketones  
under solvent-free conditions

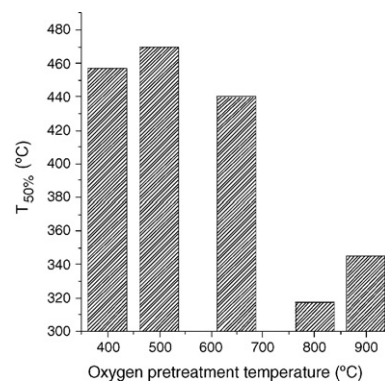


**Kun Qian, Zhiqian Jiang, Weixin Huang**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 26

Effect of oxygen treatment on the catalytic activity of Au/SiO<sub>2</sub> catalysts

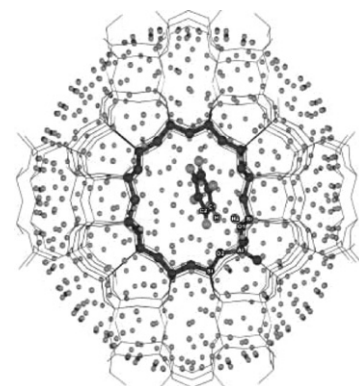
Oxygen pretreatment of Au/SiO<sub>2</sub> catalysts above 800 °C greatly enhances the catalytic activity towards CO oxidation.

**Bavornpon Jansang, Tanin Nanok, Jumras Limtrakul**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 33

Interaction of mordenite with an aromatic hydrocarbon: An embedded ONIOM study

Adsorption of benzene in the nanoporous mordenite modeled with the embedded ONIOM2 scheme.

**N. Suryakiran, P. Prabhakar, T. Srikanth Reddy, M. Srinivasulu, N. Raghavendra Swamy, Y. Venkateswarlu**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 40

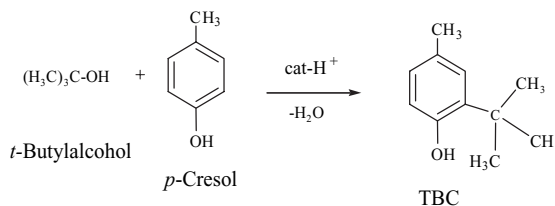
Rapid *N*-*tert*-butoxycarbonylation of amines using Bi(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O as a mild and highly efficient catalyst under solvent-free conditions

**M. Selvaraj, P.K. Sinha**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 44

Highly selective synthesis of *t*-butyl-*p*-cresol (TBC) by *t*-butylation of *p*-cresol with *t*-butyl alcohol over microporous and mesoporous catalysts

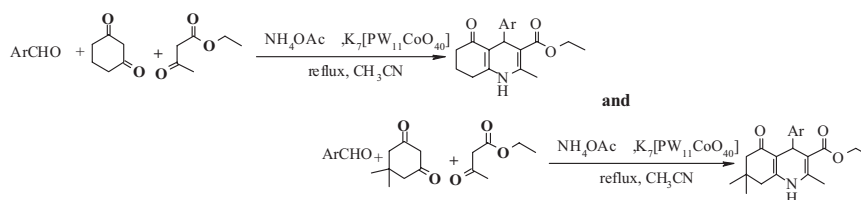
A novel mesoporous Zn–Al–MCM-41 is found to be a highly active and recyclable heterogeneous catalyst suitable for the selective synthesis of TBC by *t*-butylation of *p*-cresol with butyl alcohol having much higher acidity and activity than other catalysts, such as Al–MCM-41(21), USY, H $\beta$ , H-ZSM-5 and H-mordenite.



**Majid M. Heravi, Khadijeh Bakhtiari,  
Negar M. Javadi, Fatemeh F. Bamoharram,  
Mina Saeedi, Hossein A. Oskooie**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 50

$K_7[PW_{11}CoO_{40}]$ -catalyzed one-pot synthesis of polyhydroquinoline derivatives via the Hantzsch three component condensation

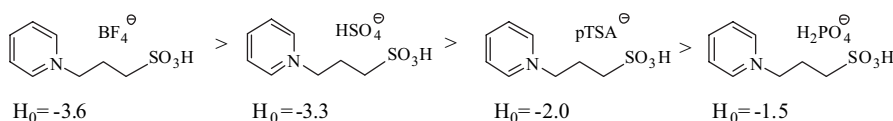


**Huabin Xing, Tao Wang, Zhenhuan Zhou,  
Youyuan Dai**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 53

The sulfonic acid-functionalized ionic liquids with pyridinium cations: Acidities and their acidity-catalytic activity relationships

The acidities and catalytic activities of sulfonic acid-functionalized ionic liquids with pyridinium cations depend on the kinds of anions. The minimum-energy geometries of SFILs manifest that the anions have strong interactions with the sulfonic acid proton. It is considered that in addition to the alkyl sulfonic acid group, the anion is likely to serve as available acid sites. Hence the acidities and catalytic activities of SFILs depend on the kinds of anions.

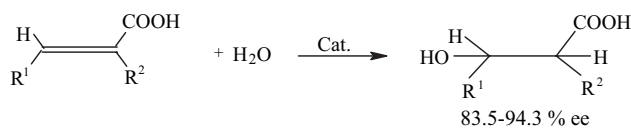


**Si-Qian Wang, Zi-Wei Wang, Lin-Chun Yang,  
Jin-long Dong, Cai-Qin Chi, Dan-Ni Sui,  
Yong-Zhao Wang, Jian-Guo Ren, Mei-Yu Hung,  
Ying-Yan Jiang**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 60

A novel efficient route for preparation of chiral  $\beta$ -hydroxycarboxylic acid: Asymmetric hydration of unsaturated carboxylic acids catalyzed by hetero-bimetallic complex wool-palladium-cobalt

A new bio-polymer heterobimetallic complex wool-Pd-Co has been found to be a novel efficient catalyst for asymmetric hydration of unsaturated carboxylic acids with high enantioselectivity by a simple and clean process under mild conditions. Chemical and optical yields are affected by some parameters, such as the (Pd + Co) content in wool-Pd-Co, the Co/Pd molar ratio, reaction time, reaction temperature and amount of water. After 5-time use of the complex, the chemical and optical yields of the products show no significant changes. Obviously, the methods provide an alternative way to produce chiral  $\beta$ -hydroxycarboxylic acids.

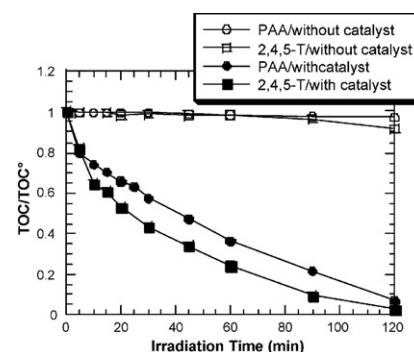


**Hemant K. Singh, Mohd Saquib,  
Malik M. Haque, Mohammad Muneer,  
Detlef W. Bahnemann**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 66

Titanium dioxide mediated photocatalysed degradation of phenoxyacetic acid and 2,4,5-trichlorophenoxyacetic acid, in aqueous suspensions

Phenoxyacetic acid (PAA) and 2,4,5-trichlorophenoxyacetic acid (2,4,5-T) undergo photomineralization in aqueous suspensions of  $TiO_2$ .

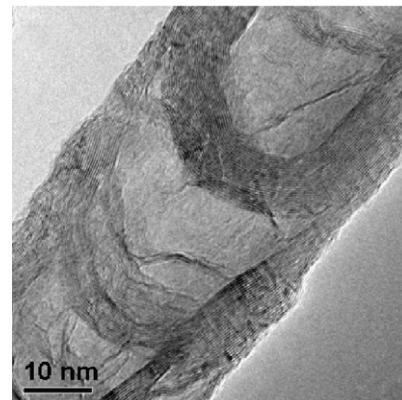


**Paul H. Matter, Eugenia Wang, Maria Arias, Elizabeth J. Biddinger, Umit S. Ozkan**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 73

Oxygen reduction reaction activity and surface properties of nanostructured nitrogen-containing carbon

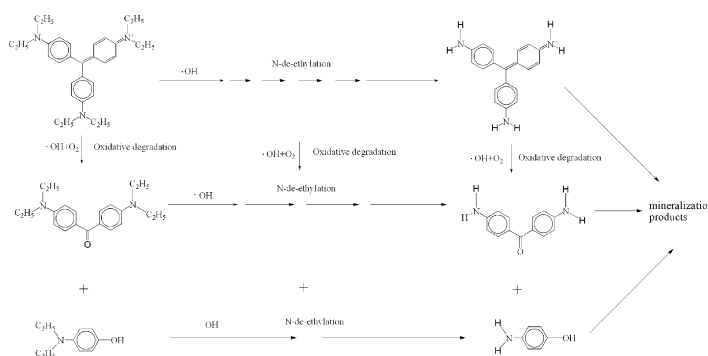
Active catalysts for the oxygen reduction reaction were prepared by growing nitrogen-containing carbon nanofibers during acetonitrile pyrolysis over Fe or Co metal particles. The particles were supported by silica or magnesia, which could subsequently be removed with KOH or HCl washing, respectively. Half-cell activity testing demonstrated comparable activity to state-of-the-art platinum catalysts. The figure is a TEM image of a fiber grown over a 2-wt% Co/MgO support.



**Chiing-Chang Chen**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 82

Degradation pathways of ethyl violet by photocatalytic reaction with ZnO dispersions

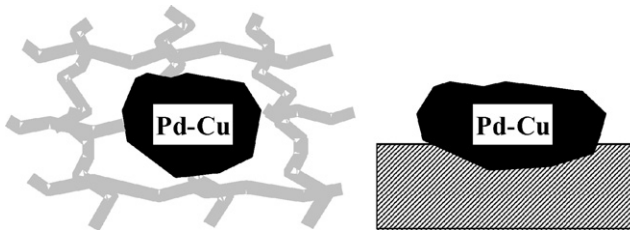


**Dana Gašparovičová, Milan Králík, Milan Hronec, Zuzana Vallušová, Hannelore Vinek, Benedetto Corain**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 93

Supported Pd–Cu catalysts in the water phase reduction of nitrates: Functional resin *versus* alumina

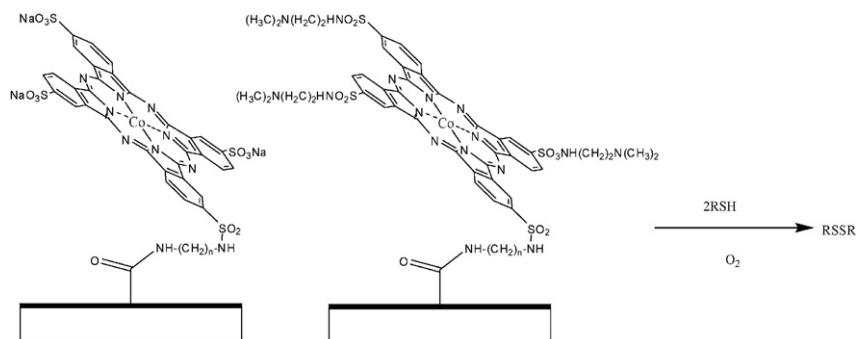
A performance of bimetallic Pd–Cu catalysts supported on functional gel type resin and gamma-alumina in the liquid-phase hydrogenation of nitrates has been compared. Pd–Cu alloys (alumina support) or isolated domains of metallic palladium and copper, if any, were found by means of TEM and XRPD. The Pd–Cu catalysts supported on alumina were more active, but less selective to nitrogen than their resin type counterparts. In spite of smaller metal particles generated inside the polymer framework, this type of catalyst proved to be more stable than that supported on  $\gamma$ -alumina.



**Victor N. Nemykin, Ann E. Polshyna, Svetlana A. Borisenkova, Vladimir V. Strelko**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 103

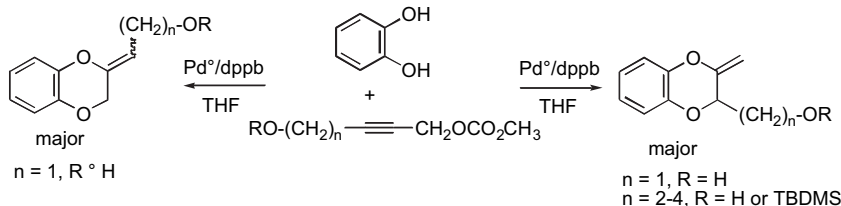
Preparation, characterization, and catalytic activity of synthetic carbon-supported (phthalocyaninato) cobalt-containing complexes in dodecane-1-thiol oxidation reaction



**Norbert Dominczak, Paul Lhoste,  
Boguslaw Kryczka, Denis Sinou**

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 110

Palladium-catalyzed heteroannulation of catechol with functionalized propargylic carbonates: Influence of the functional group on the regioselectivity of the cyclization

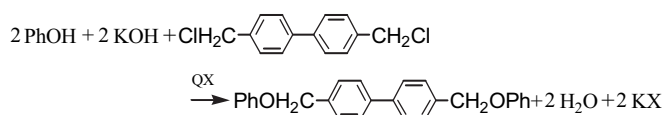


**Maw-Ling Wang, Ze-Fa Lee**

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 119

Reaction of 4,4'-bis(chloromethyl)-1,1'-biphenyl and phenol in two-phase medium via phase-transfer catalysis

The overall reaction of the etherification of 4,4'-bis(chloromethyl)-1,1'-biphenyl with phenol is Tetra-*n*-butylammonium bromide was used as a liquid-liquid phase-transfer catalyst (LL-PTC, Q). Potassium phenoxide ( $\text{PhO}^- \text{K}^+$ ) was synthesized *in situ* directly by reacting phenol with potassium hydroxide in the aqueous phase. 4,4'-(Chloromethylphenoxy)methyl)-1,1'-biphenyl was first synthesized by reacting phenoxide with 4,4'-bis(chloromethyl)-1,1'-biphenyl in an organic solvent. Afterward, 4,4'-bis(phenoxy)methyl)-1,1'-biphenyl was produced by further reacting phenoxide with 4,4'-(chloromethylphenoxy)methyl)-1,1'-biphenyl.



**Tarek M. Salama, Zeinhom M. El-Bahy,  
Farouk I. Zidan**

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 128

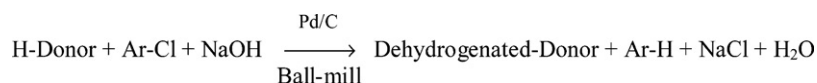
Aqueous  $\text{H}_2\text{O}_2$  as an oxidant for CO over Pt- and Au-NaY catalysts

The oxidation of carbon monoxide with aqueous hydrogen peroxide was carried out over Pt- and Au-NaY catalysts, that were prepared by the impregnation of NaY zeolite ( $\text{Si}/\text{Al} = 5.6$ ,  $S_{\text{BET}} = 910 \text{ m}^2/\text{g}$ ) with aqueous solutions of tetramine platinum(II) nitrate and hydrogen tetrachloroaurate trihydrate, respectively. The Pt- and Au-NaY catalysts exhibited high activity at relatively low temperatures as low as 303 K in the  $\text{CO}-\text{H}_2\text{O}_2$  reaction. Pt-NaY was compared favorably with Au-NaY at similar reaction conditions, where the specific reaction rate constant,  $K_m$ , over Pt-NaY was five times of magnitude higher than that of Au-NaY at 323 K. These data were confirmed by the values of activation energy evaluated from Arrhenius plots. The Pt-NaY was reduced in flowing  $\text{H}_2$  at 623 K for 2 h. The catalytic activity of reduced Pt-NaY was about 44 times more active than that of analogous unreduced catalyst at 303 K. The catalytic activity of Au-NaY was greatly affected by thermal treatment. A higher  $K_m$  value was obtained at 353 K over Au-NaY, exceeding this temperature led to a decrease in activity due to sintering of Au particles. It is proposed that a dual Au(0)/Au(I) site is necessary to catalyze the reaction, where, Au(0) accelerates the  $\text{H}_2\text{O}_2$  decomposition and the CO adsorption capability was enhanced on Au(I) site.

**Ilan Pri-Bar, Brian R. James**

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 135

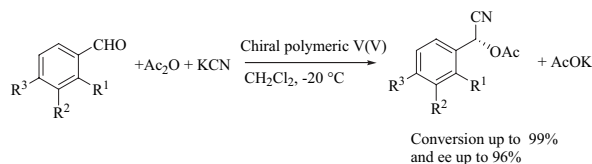
Mechanochemical, solvent free, palladium-catalyzed hydrodechlorination of chloroaromatic hydrocarbons



Noor-ul H. Khan, Santosh Agrawal,  
Rukhsana I. Kureshy, Sayed H.R. Abdi,  
Vishal J. Mayani, Raksh V. Jasra

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 140

Easily recyclable polymeric V(V) salen complex for  
the enantioselective *O*-acetyl cyanation of aldehydes

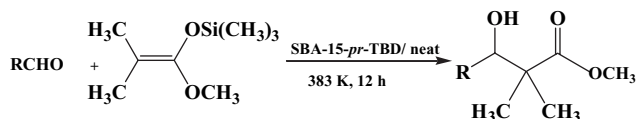


Rajendra Srivastava

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 146

An efficient, eco-friendly process for aldol and  
Michael reactions of trimethylsilyl enolate over  
organic base-functionalized SBA-15 catalysts

1,5,7-Triazabicyclo[4.4.0]dec-5-ene (TBD, a bicyclic guanidine base) functionalized SBA-15 was found to be an efficient catalyst for Aldol reaction of trimethylsilyl enolate with aldehydes. Both aryl aldehydes and alkyl aldehydes provided the aldol product in good yields. The applicability of this catalyst was extended to Michael reaction and in the synthesis of quaternary carbon. This novel heterogeneous catalyst offer several attractive advantages over soluble base catalysts such as high catalyst activity under mild reaction condition, easy recovery of the catalyst and reusability of the catalyst.

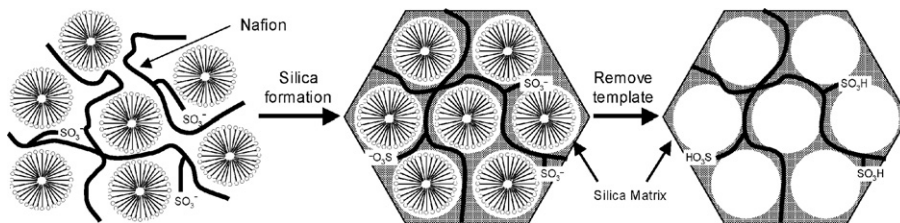


Masahiro Fujiwara, Kumi Shiokawa,  
Yingchun Zhu

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 153

Preparation of mesoporous silica/polymer sulfonate  
composite materials

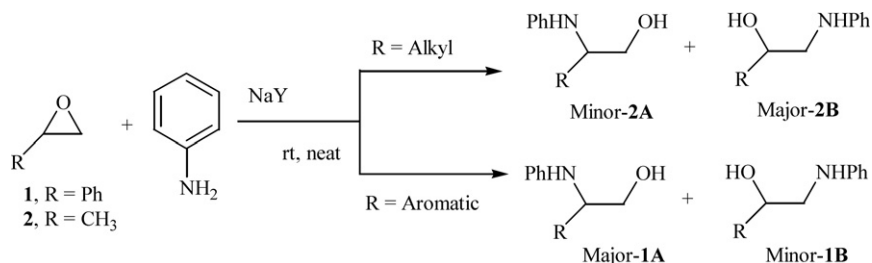
Mesoporous silica/polymer sulfonate composite materials are prepared by mixing hexadecyltrimethylammonium bromide, polymer sulfonates and tetraethoxysilane in aqueous solution and used as catalysts for  $\alpha$ -methylstyrene dimerization and Friedel–Crafts alkylation reaction of aromatics.



Rukhsana Ilyas Kureshy, Surendra Singh,  
Noor-ul Hasan Khan, Sayed Hasan Razi Abdi,  
Eringathodi Suresh, Raksh Vir Jasra

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 162

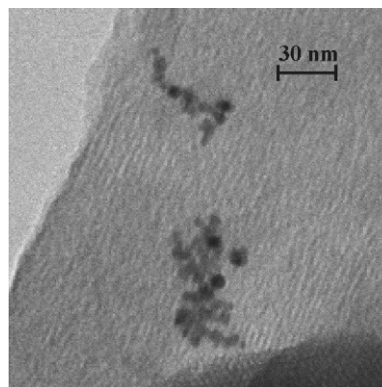
Efficient method for ring opening of epoxides with  
amines by NaY zeolite under solvent-free conditions



Ágnes Mastalir, Bulcsú Rác, Zoltán Király,  
Árpád Molnár

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 170

In situ generation of Pd nanoparticles in MCM-41  
and catalytic applications in liquid-phase alkyne  
hydrogenations

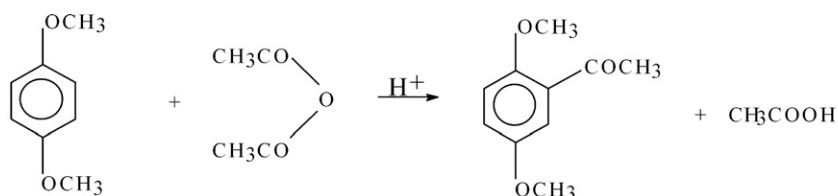


Ganapati D. Yadav, Ketan P. Pimparkar

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 179

Insight into Friedel-Crafts acylation of 1,4-  
dimethoxybenzene to 2,5-dimethoxyacetophenone  
catalysed by solid acids—mechanism, kinetics and  
remedies for deactivation

Acylation of 1,4 dimethoxybenzene with acetic anhydride is studied systematically over several solid acids  
and the ion exchange resins were found to be superior.



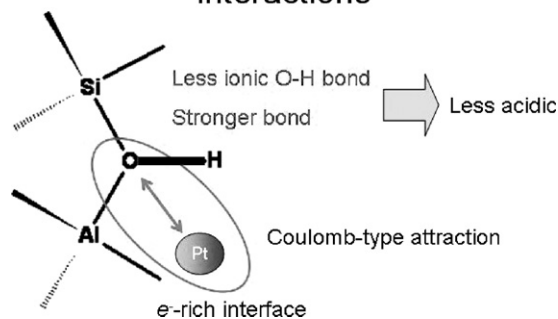
1,4- Dimethoxybenzene(A) Acetic anhydride(B) 2,5-Dimethoxyacetophenone (C) Acetic acid (D)

I. Villegas, D. Kubička, H. Karhu,  
H. Österholm, N. Kumar, T. Salmi,  
D.Yu. Murzin

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 192

On the mutual interactions between noble metal  
crystallites and zeolitic supports and their impacts  
on catalysis

### Pt – (zeolitic) support mutual interactions

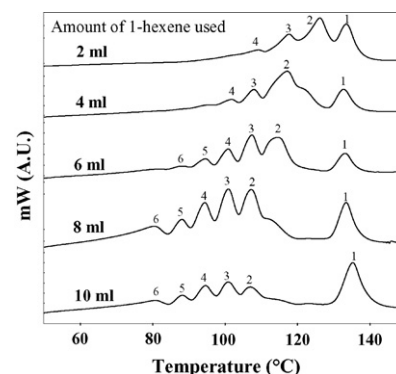


Hai Woong Park, Jin Suk Chung, Seong Soo  
Lim, In Kyu Song

*Journal of Molecular Catalysis A: Chemical* 264  
(2007) 202

Chemical composition distributions and microstructures of ethylene–hexene copolymers produced by a  
*rac*-Et(Ind)<sub>2</sub>ZrCl<sub>2</sub>/TiCl<sub>4</sub>/MAO/SMB catalyst

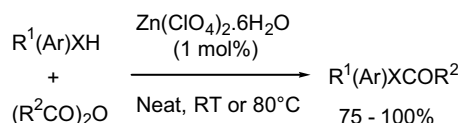
Ethylene–hexene copolymers were produced by a  
*rac*-Et(Ind)<sub>2</sub>ZrCl<sub>2</sub>/TiCl<sub>4</sub>/MAO(methylaluminoxane)/SMB(silica-magnesium bisupport) catalyst by  
varying the amount of 1-hexene used. It was found  
that the number of chemical composition distribution  
(CCD) peaks was increased and the short chain  
branches were distributed over the lower temperature  
region with increasing 1-hexene content.



**Shivani, Rajesh Gulhane, Asit K. Chakraborti**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 208

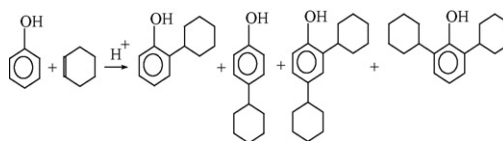
Zinc perchlorate hexahydrate [Zn(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O] as acylation catalyst for poor nucleophilic phenols, alcohols and amines: Scope and limitations

**Nikunj Bhatt, Anjali Patel**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 214

Liquid phase cyclohexylation of phenol with cyclohexene using 12-tungstosilicic acid supported onto different supports

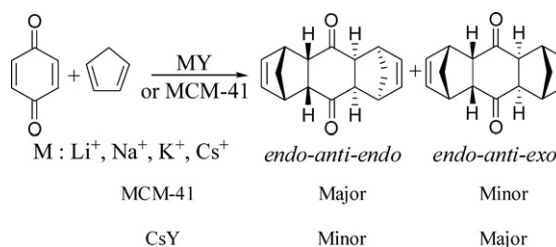
Acid catalysts having 30% loading of 12-tungstosilicic acid onto hydrous zirconia and neutral alumina were synthesized by impregnation method. The synthesized catalysts were evaluated for the cyclohexylation reactions of phenol, which were carried out by varying different parameters. The activities of both the catalyst were compared in order to see the effect of nature of the support.

**Gholamreza Mashayekhi, Mehdi Ghandi, Faezeh Farzaneh, Mansour Shahidzadeh, Heydar Mahmoudi Najafi**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 220

Experimental and semiempirical studies of effect of MCM-41 and cation exchanged zeolite Y on rate enhancement and diastereoselectivity of Diels–Alder reaction of *p*-benzoquinone and some derivatives with cyclopentadiene

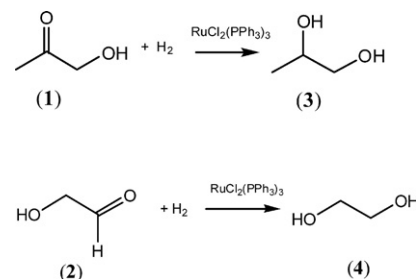
The 2:1 adducts of Diels–Alder reaction of cyclopentadiene with *p*-benzoquinone catalyzed by MCM-41 and alkali cation exchanged zeolite Y characterized as *endo-anti-endo* and *endo-anti-exo* as the major products, respectively, were rationalized by semiempirical calculations using PM5 method.

**F.H. Mahfud, F. Ghijsen, H.J. Heeres**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 227

Hydrogenation of fast pyrolysis oil and model compounds in a two-phase aqueous organic system using homogeneous ruthenium catalysts

The use of homogeneous ruthenium catalysts to hydrogenate pyrolysis oil is reported. The hydrogenation experiments were performed at mild conditions (40 bar, 90 °C) using a biphasic system (water/toluene) and RuCl<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub> as the toluene soluble catalyst. Significant reductions in the amounts of 1-hydroxy-2-propanone (**1**) and 1-hydroxy-2-ethanal (**2**), present in pyrolysis oil in significant amounts, were observed. Model studies showed that **1** and **2** are selectively hydrogenated to 1,2-propanediol and 1,2-ethanediol, respectively.



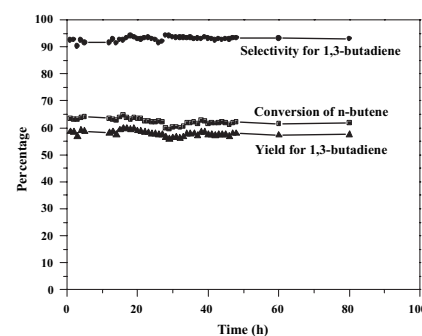


**Ji Chul Jung, Heesoo Kim, Young-Min Chung,  
Tae Jin Kim, Seong Jun Lee, Seung-Hoon Oh,  
Yong Seung Kim, In Kyu Song**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 237

Unusual catalytic behavior of  $\beta$ - $\text{Bi}_2\text{Mo}_2\text{O}_9$  in the oxidative dehydrogenation of *n*-butene to 1,3-butadiene

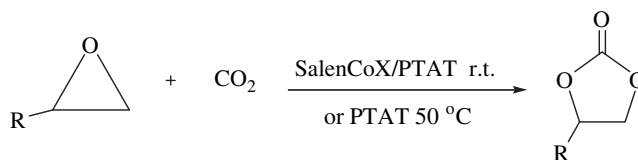
A  $\beta$ - $\text{Bi}_2\text{Mo}_2\text{O}_9$  catalyst was prepared by a co-precipitation method for use in the oxidative dehydrogenation of *n*-butene. It was found that the  $\beta$ - $\text{Bi}_2\text{Mo}_2\text{O}_9$  catalyst showed a high and stable catalytic performance without catalyst deactivation, in spite of its thermal instability and low oxygen mobility.



**Tao Chang, Huanwang Jing, Lili Jin,  
Wenyuan Qiu**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 241

Quaternary onium tribromide catalyzed cyclic carbonate synthesis from carbon dioxide and epoxides



**J. Das, K.M. Parida**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 248

Heteropoly acid intercalated Zn/Al HTlc as efficient catalyst for esterification of acetic acid using *n*-butanol

The effect of various reaction parameters such as molar ratio of the reactants, temperature, time and catalyst dose, etc. on the conversion of acetic acid was studied and the findings are discussed. The 15 wt.% MPA intercalated sample shows highest conversion (84.15%) with almost 100% selectivity for *n*-butyl acetate.

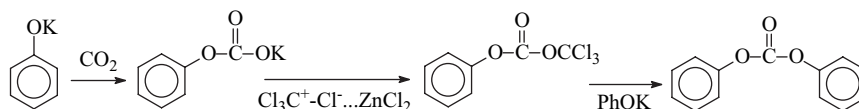


**Zhenhuan Li, Zhangfeng Qin**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 255

Synthesis of diphenyl carbonate from phenol and carbon dioxide in carbon tetrachloride with zinc halides as catalyst

Synthesis of diphenyl carbonate (DPC) from phenol and  $\text{CO}_2$  has been explored in  $\text{CCl}_4$  with zinc halides as catalyst. DPC yield and selectivity are influenced by the catalyst usage, reaction temperature,  $\text{CO}_2$  pressure and initial composition of reactants.  $\text{ZnCl}_2$  as Lewis acid exhibits high catalytic activity for DPC synthesis. Based on the experimental observation, possible reaction scheme has been proposed.

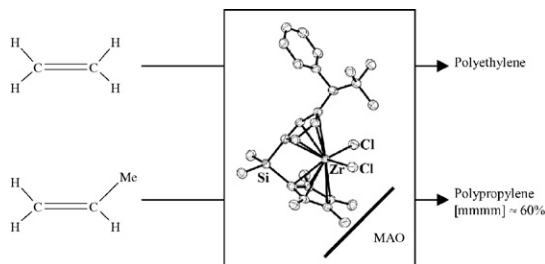


**Santiago Gómez-Ruiz, Sanjiv Prashar, Luis F. Sánchez-Barba, Dorian Polo-Cerón, Mariano Fajardo, Antonio Antiñolo, Antonio Otero, Miguel A. Maestro, César J. Pastor**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 260

Synthesis and catalytic applications of  $C_1$  symmetric group 4 *ansa*-metallocene complexes

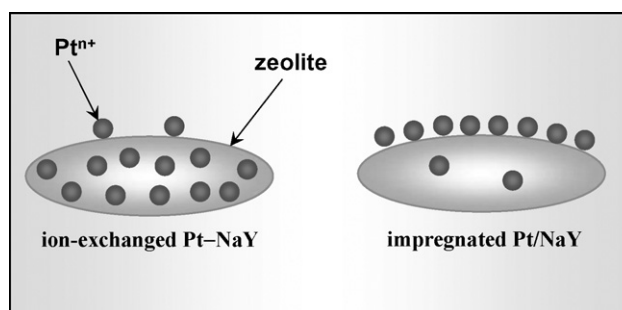
The preparation and characterization of new group 4 *ansa*-metallocene complexes containing chiral substituents and their role as catalysts in ethylene and propylene polymerization are described.



**Kristina Chakarova, Konstantin Hadjiivanov, Genoveva Atanasova, Krassimir Tenchev**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 270

Effect of preparation technique on the properties of platinum in NaY zeolite: A study by FTIR spectroscopy of adsorbed CO

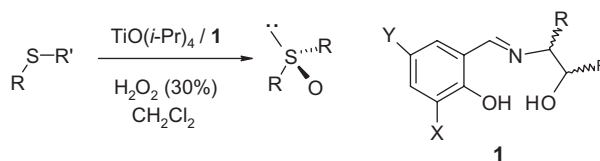


**Konstantin P. Bryliakov, Evgenii P. Talsi**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 280

Asymmetric oxidation of sulfides with  $H_2O_2$  catalyzed by titanium complexes with aminoalcohol derived Schiff bases

Sulfoxidation catalysts generated in situ from titanium(IV) isopropoxide and enantiopure Schiff bases promote the enantioselective oxidation of alkyl aryl sulfides to the corresponding sulfoxides with over 90% chemoselectivity and up to 60% ee at low catalyst loadings (<1 mol%), 30% aqueous hydrogen peroxide being the terminal oxidant.



**M. Narasimhulu, T. Srikanth Reddy, K. Chinni Mahesh, S. Malla Reddy, A. Vijender Reddy, Y. Venkateswarlu**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 288

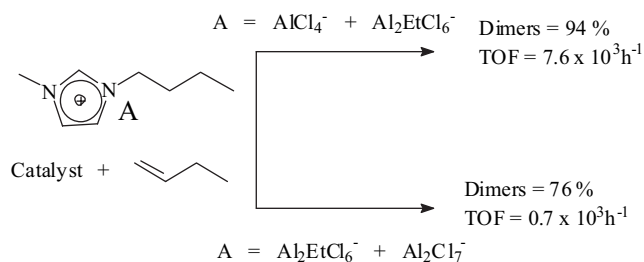
Lanthanum(III) nitrate hexahydrate or gadolinium(III) chloride hexahydrate catalyzed one-pot synthesis of  $\alpha$ -amino nitriles



**Daniel Thiele, Roberto Fernando de Souza**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 293

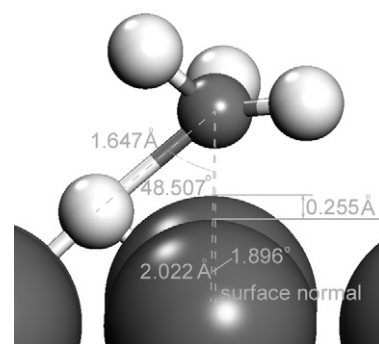
The role of aluminum species in biphasic butene dimerization catalyzed by nickel complexes

**Yi-An Zhu, Ying-Chun Dai, De Chen, Wei-Kang Yuan**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 299

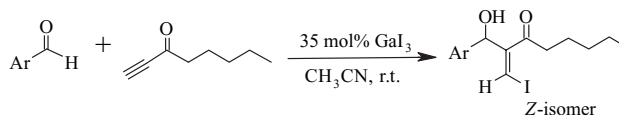
First-principles calculations of CH<sub>4</sub> dissociation on Ni(1 0 0) surface along different reaction pathways

First-principles calculations based on density functional theory and the generalized gradient approximation have been used to study the adsorption and dissociation of CH<sub>4</sub> on Ni(1 0 0) surface. Three reaction pathways starting from different CH<sub>4</sub> orientations are considered. Because the energy barriers for the different reaction pathways take similar values, the CH<sub>4</sub> orientation has a minor effect on the reactivity.

**J.S. Yadav, B.V.S. Reddy, Manoj K. Gupta, Sushil K. Pandey**

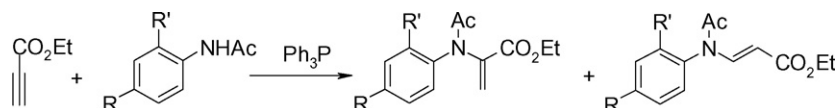
*Journal of Molecular Catalysis A: Chemical* 264 (2007) 309

Gallium(III) iodide-promoted stereoselective aldol coupling of  $\alpha,\beta$ -acetylenic ketones

**Issa Yavari, Norollah Hazeri, Malek T. Maghsoodlou, Sanaz Souri**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 313

Ph<sub>3</sub>P catalyzed efficient synthesis of ethyl 2-(acetylanilino)-acrylates and ethyl (E)-3-(acetylanilino)-2-propenoates by nucleophilic addition to ethyl propiolate



**Majid M. Heravi, Tina Benmorad, Khadijeh Bakhtiari, Fatemeh F. Bamoharram, Hossein H. Oskooie**

*Journal of Molecular Catalysis A: Chemical* 264 (2007) 318

$H_{3+x}PMo_{12-x}V_xO_{40}$  (heteropolyacids)-catalyzed regioselective nitration of phenol to *o*-nitrophenol in heterogeneous system

