

## Contents

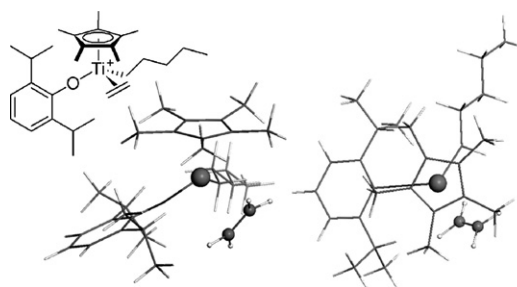
### Articles

**Kotohiro Nomura, Jingyu Liu,  
Sudhakar Padmanabhan,  
Boonyarach Kitiyanan**

*Journal of Molecular Catalysis A: Chemical 267*  
(2007) 1

Nonbridged half-metallocenes containing anionic ancillary donor ligands: New promising candidates as catalysts for precise olefin polymerization

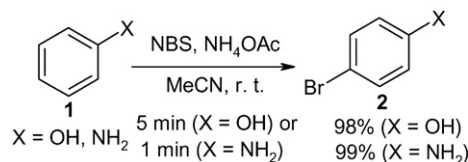
Recent examples for nonbridged group 4 half-metallocenes containing anionic donor ligands of the type, Cp'MX<sub>2</sub>(L), as catalysts for precise olefin polymerization have been reviewed. These catalysts displayed unique characteristics especially for ethylene copolymerizations, affording new polyolefins that can not be prepared by ordinary catalysts; ligand modifications are the key for precise olefin (co)polymerization.



**Biswanath Das, Katta Venkateswarlu,  
Anjoy Majhi, Vidavalur Siddaiah,  
Kongara Ravinder Reddy**

*Journal of Molecular Catalysis A: Chemical 267*  
(2007) 30

A facile nuclear bromination of phenols and anilines using NBS in the presence of ammonium acetate as a catalyst

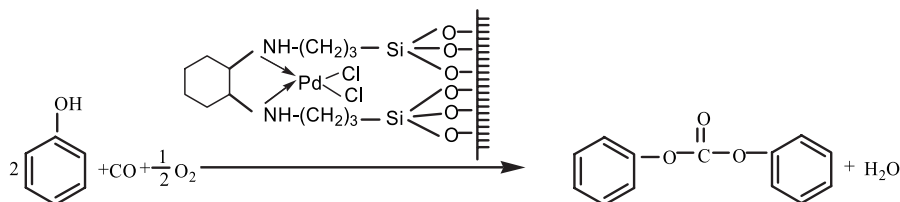


**Guozhi Fan, Jiao Huang, Zhiqiang Li, Tao Li,  
Guangxing Li**

*Journal of Molecular Catalysis A: Chemical 267*  
(2007) 34

Palladium complexes anchored on silica functionalized by 1,2-diaminocyclohexane: Preparation and catalytic application

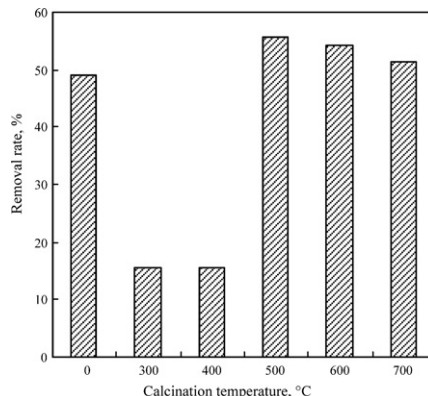
Palladium complexes anchored on organic–inorganic hybrid materials modified by 1,2-diaminocyclohexane were prepared. The heterogeneous catalyst proved to be an excellent catalyst for the oxidative carbonylation of phenol to diphenyl carbonate (DPC).



**Yixin Yang, Jun Ma, Qingdong Qin, Xuedong Zhai**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 41

Degradation of nitrobenzene by nano-TiO<sub>2</sub> catalyzed ozonation

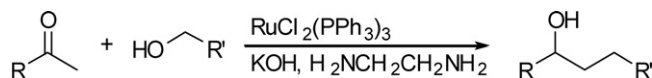


**Chan Sik Cho**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 49

Ruthenium-catalyzed reductive coupling between ketones and primary alcohols in the presence of ethylenediamine

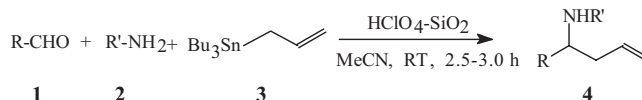
An atom economical ruthenium-catalyzed reductive cross-coupling between ketones and primary alcohols in the presence of ethylenediamine and KOH is described.



**Lingaiah Nagarapu, Venkateswarlu Paparaju, Gopal Pathuri, Srinivas Kantevari, Rupa Rani Pakkuru, Radhika Kamalla**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 53

HClO<sub>4</sub>-SiO<sub>2</sub> as a novel and recyclable catalyst for the one-pot synthesis of homoallylic amines

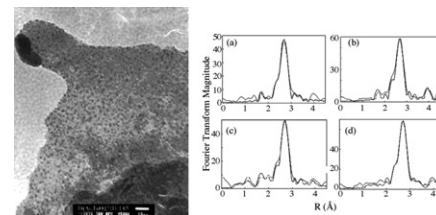


**Suresh K. Bhargava, Deepak B. Akolekar, Garry Foran**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 57

Investigations on gold nanoparticles supported on rare earth oxide catalytic materials

Supported gold nanoparticles rare earth (europium, dysprosium, samarium oxide, neodymium, gadolinium oxide and lanthanum oxide) materials were prepared and characterised by routine and sophisticated techniques. Au L<sub>3</sub>-edge X-ray absorption spectroscopic measurements were carried out over a series of rare earth materials containing gold nanoparticles. The size of gold nanoparticles varied in the range of ~2 to 6 nm in the Eu/Dy/Sm/Nd/Gd/La materials in obtaining critical information about the atomic distances, bonding and neighbouring environment for gold atoms. These materials possess medium surface area between 29 and 41 m<sup>2</sup>/g with the high phase purity and crystallinity of the support (Eu/Dy/Sm/Nd/Gd/La) materials.

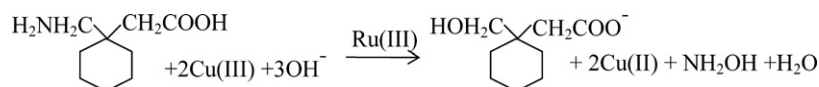


**Shivamurti A. Chimatadar, T. Basavaraj,  
Kiran A. Thabaj, Sharanappa T. Nandibewoor**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 65

Ruthenium(III) catalysed oxidation of gabapentin  
(neurontin) by diperiodatocuprate(III) in aqueous  
alkaline medium—A kinetic and mechanistic study

The mechanistic investigation of oxidation of neuroleptic drug gabapentin by diperiodatocuprate(III) (DPC) has been carried out in the presence of minute amounts of ruthenium(III) catalyst in an aqueous alkaline medium. The reaction is found to be first order with respect to both DPC and ruthenium(III) concentrations and less than unity order with respect to gabapentin concentrations. The active species of Cu(III) and Ru(III) in the reaction medium are  $[\text{Cu}(\text{OH})_2(\text{H}_3\text{IO}_6)(\text{H}_2\text{IO}_6)]^{4-}$  and  $[\text{Ru}(\text{H}_2\text{O})_5(\text{OH})]^{2+}$ , respectively.

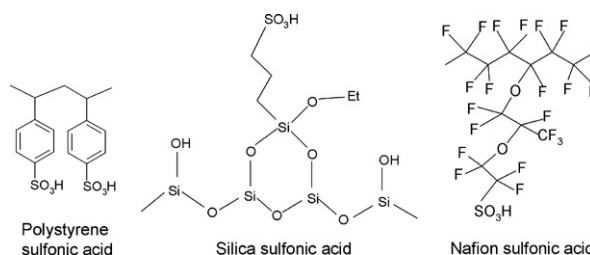


**P.F. Siril, A.D. Davison, J.K. Randhawa,  
D.R. Brown**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 72

Acid strengths and catalytic activities of sulfonic  
acid on polymeric and silica supports

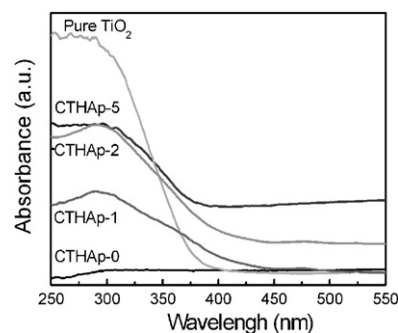
The acidic and catalytic properties of sulfonic acids (structure given below) supported on polystyrene, on silica (via propyl and phenyl tethers) and on a fluorinated hydrocarbon polymer (Nafion) are compared. Adsorption of ammonia from a flowing carrier gas stream was used to characterise the surface acidity of these catalysts and the catalytic activities for isomerisation of  $\alpha$ -pinene have been explained on the basis of acidity characterisation.



**Anmin Hu, Ming Li, Chengkang Chang,  
Dali Mao**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 79

Preparation and characterization of a titanium-  
substituted hydroxyapatite photocatalyst

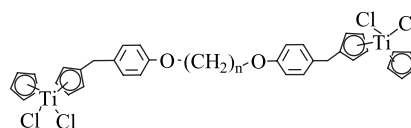


**Xiaohui Xiao, Junquan Sun, Xu Li,  
Hongfeng Li, Yanguang Wang**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 86

Binuclear titanocenes linked by the bridge combination of rigid and flexible segment: Synthesis and their use as catalysts for ethylene polymerization

Five novel binuclear titanocenes  $(\text{CpTiCl}_2)_2[(\text{C}_5\text{H}_4)\text{CH}_2(p\text{-C}_6\text{H}_4)\text{O}(\text{CH}_2)_n\text{O}(\text{C}_6\text{H}_4\text{-}p)\text{-CH}_2(\text{C}_5\text{H}_4)]$  ( $n = 2-6$ ) (**16-20**) with the bridge combination of rigid and flexible segment were synthesized. In the presence of methylaluminoxane, the behaviors of these complexes toward ethylene polymerization were investigated. The results show that their catalytic behaviors are highly dependent on the length of flexible segment and polymerization conditions.



**16**( $n=2$ ), **17**( $n=3$ ), **18**( $n=4$ ), **19**( $n=5$ ), **20**( $n=6$ )

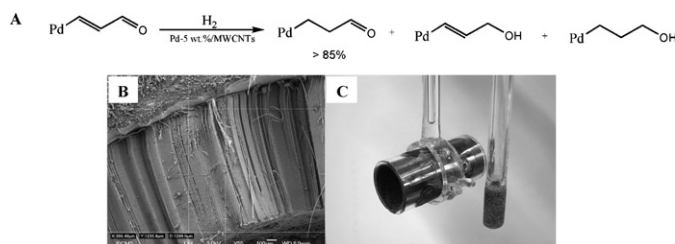
Structure of the catalyst 16-20

**Izabela Janowska, Gauthier Winé,  
Marc-Jacques Ledoux, Cuong Pham-Huu**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 92

Structured silica reactor with aligned carbon nanotubes as catalyst support for liquid-phase reaction

The synthesis of aligned (B) and strongly attached multi-walled carbon nanotubes on the wall of a silica reactor, which can be efficiently used as a catalyst support in liquid-phase reactions was executed. The CNTs/SiO<sub>2</sub> tube (C) was directly used as mechanical stirrer in the selective hydrogenation of cinnamaldehyde using palladium as an active phase (A). The selectivity towards the hydrocinnamaldehyde, i.e. C=C bond hydrogenation, remained high and constant regardless of the level of conversion, i.e. selectivity of 90% at a conversion of about 80%.

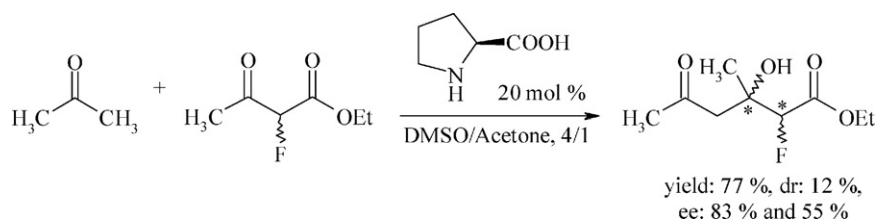


**Gábor London, György Szöllösi, Mihály Bartók**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 98

Organocatalytic direct aldol reaction between acetone and  $\alpha$ -substituted  $\beta$ -keto esters

The L-proline catalyzed direct aldol addition of acetone on  $\alpha$ -fluorinated  $\beta$ -keto esters afforded  $\delta$ -keto- $\beta$ -hydroxy- $\alpha$ -fluoro esters in high yields. In the reaction of ethyl 2-fluoroacetoacetate good enantiomeric excesses, up to 83%, coupled with low diastereoselectivities were obtained.

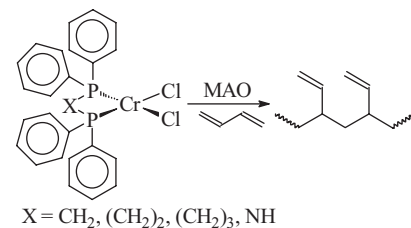


**Giovanni Ricci, Aldo Boglia, Tiziano Motta**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 102

Synthesis of new Cr(II) complexes with bidentate phosphine ligands and their behavior in the polymerization of butadiene. Influence of the phosphine bite angle on catalyst activity and stereoselectivity

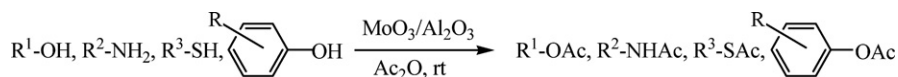
Some new chromium(II) complexes obtained by reacting CrCl<sub>2</sub>(thf) with various bidentate phosphines [bis(diphenylphosphino)methane (dppm); 1,2-bis(diphenylphosphino)ethane (dppe); 1,3-bis(diphenylphosphino)propane (dppp); bis(diphenylphosphino)amine (dppa)] were used, in combination with MAO, for polymerizing butadiene. They were found to be in some cases extremely active and they gave predominantly 1,2-polybutadienes (1,2 content >85%) having different tacticity (syndiotactic or predominantly isotactic) depending on the phosphine ligand bonded to the chromium atom.



**Jomy K. Joseph, Suman L. Jain, Bir Sain**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 108

Alumina supported MoO<sub>3</sub> as a highly efficient and recyclable heterogeneous catalyst for the chemoselective acetylation of alcohols, phenols amines and thiols with acetic anhydride under solvent free conditions

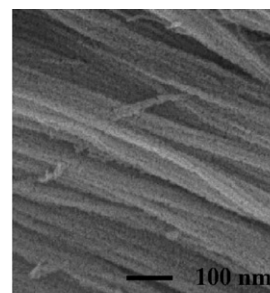


**Song-Taek Oh, Jae-Suk Choi, Han-Su Lee, Lianhai Lu, Heock-Hoi Kwon, In Kyu Song, Jae Jeong Kim, Ho-In Lee**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 112

H<sub>2</sub>O-controlled synthesis of TiO<sub>2</sub> with nanosized channel structure through *in situ* esterification and its application to photocatalytic oxidation

TiO<sub>2</sub> was synthesized by hydrolysis of titanium precursor with water produced from *in situ* esterification between acetic acid and polymers containing hydroxyl group. Prepared TiO<sub>2</sub> had regular channel structure with large surface area and pore size resulted from organic–inorganic interaction induced by esterification. By tuning the structural properties, more active TiO<sub>2</sub> for cyanide and 2-isopropyl-6-methyl-4-pyrimidinol decompositions than commercial photocatalyst was obtained.



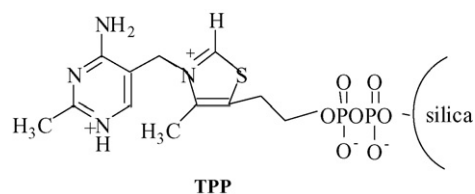
FE-SEM image of TiO<sub>2</sub> with characteristic channel structure

**Aggelos Stamatis, Gerasimos Malandrinos, Ian S. Butler, Nick Hadjiliadis, Maria Louloudi**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 120

Intermediates of thiamine catalysis immobilized on silica surface as active biocatalysts for  $\alpha$ -ketoacid decarboxylation

Two ‘active aldehyde’ intermediates of thiamine catalysis have been immobilized on a silica surface by a convenient method *via* their phosphate groups. These bio-composite materials have been evaluated as catalysts for pyruvate and benzoyl-formate decarboxylation in either the presence or not of an aldehyde additive. They are stable and very effective catalysts for the production of 2-hydroxy-ketones, acetoin and benzoin. Considering our results, possible catalytic pathways are suggested.

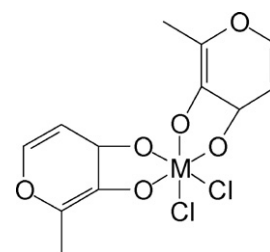


**Nara R. de S. Basso, Paula P. Greco, Carlos L.P. Carone, Paolo R. Livotto, Lílian M.T. Simplicio, Zênis N. da Rocha, Griselda B. Galland, João H.Z. dos Santos**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 129

Reactivity of zirconium and titanium alkoxides bidentate complexes on ethylene polymerization

Catalyst activity of zirconium and titanium complexes bearing bidentate ligands were evaluated in ethylene polymerization at different experimental conditions with methylaluminoxane (MAO) as the cocatalyst. According to <sup>1</sup>H NMR analysis, two stereoisomers are present for the zirconium complex. The complexes reactivity and stability were also monitored by cyclic voltammetry.

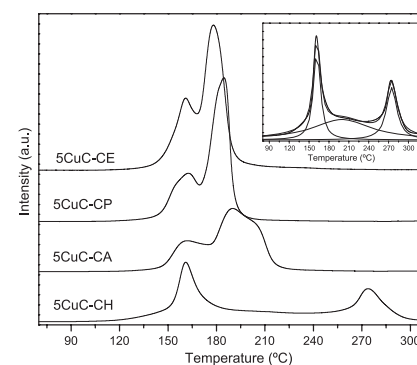


**Zhigang Liu, Renxian Zhou, Xiaoming Zheng**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 137

Comparative study of different methods of preparing CuO-CeO<sub>2</sub> catalysts for preferential oxidation of CO in excess hydrogen

The CuO-CeO<sub>2</sub> catalyst prepared by the chelating method is most active in preferential oxidation of CO. CO conversion over CuO-CeO<sub>2</sub> catalysts prepared by the chelating method is 99.6% at the temperature of 120 °C, while CO conversions over the CuO-CeO<sub>2</sub> catalysts prepared by the coprecipitation and critical-phase drying methods cannot reach 99% and that over the CuO-CeO<sub>2</sub> catalysts prepared by the citric acid method is 99.2% at 160 °C. TPR, XRD and UV Raman results show that the chelating method enhances the formation of defects of ceria and produces a synergic effect between the cycle of Cu<sup>1+</sup>/Cu<sup>2+</sup> and that of Ce<sup>3+</sup>/Ce<sup>4+</sup>, which is beneficial to the improvement of the performance of CuO-CeO<sub>2</sub> catalysts.

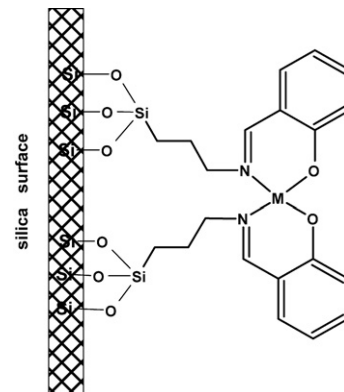


**Saptarshi Ray, Selwyn F. Mapolie,  
James Darkwa**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 143

Catalytic hydroxylation of phenol using immobilized  
late transition metal salicylaldimine complexes

Late transition metal complexes of salicylaldimine ligands immobilized on amorphous silica and MCM-41 were used as catalysts in the hydroxylation of phenol in the presence of hydrogen peroxide. Product selectivity was shown to be highly dependent on the type of support employed.

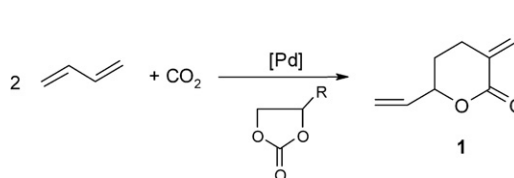


**Arno Behr, Philip Bahke, Ben Klinger,  
Marc Becker**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 149

Application of carbonate solvents in the telomerisation  
of butadiene with carbon dioxide

The chemical use of carbon dioxide as  $C_1$ -building block and supercritical solvent is becoming more and more interesting for research and industry. Carbon dioxide is a major cause of the so-called greenhouse effect, leading possibly to changes in climate. For this reason and because of the fact that carbon dioxide is a cheap and nearly unlimited  $C_1$ -building block the chemical use of  $CO_2$  is of great interest. Accounting political demands it can be assumed that the intensity of research and the interest of industry will increase. In the reaction of carbon dioxide with 1,3-butadiene it is possible to synthesize the very interesting  $\delta$ -lactone 2-ethylidene-6-heptene-5-olide under very mild reaction-conditions. By the substitution of the formerly used toxic acetonitrile with cyclic carbonates the process is now free of hazardous solvents.

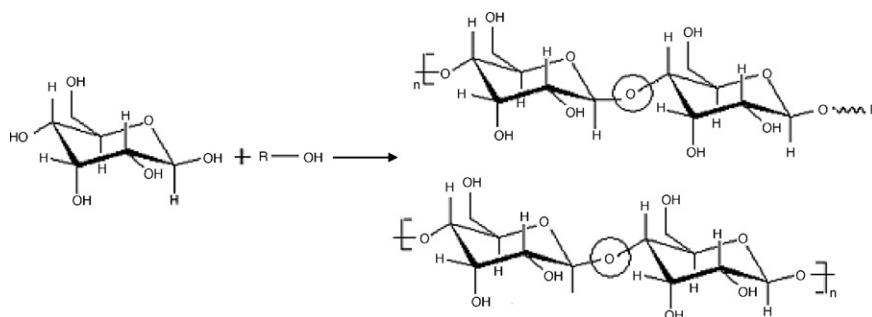


**Nivedita S. Chaubal, Vishal Y. Joshi,  
Manohar R. Sawant**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 157

Selective synthesis of alky poly- $\beta$ -D-glucopyranoside  
over mixed metal oxide

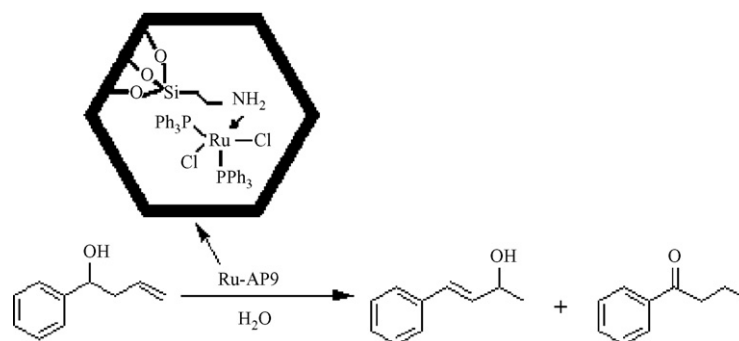
A simple synthesis of alkyl poly- $\beta$ -D-glucopyranoside performed using heterogeneous mixed metals oxides of spinel lattice to understand glycosylation mechanism over the surface of solid catalyst.



**Ying Wan, Fang Zhang, Yunfeng Lu, Hexing Li**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 165

Immobilization of Ru(II) complex on functionalized  
SBA-15 and its catalytic performance in aqueous  
homoallylic alcohol isomerization

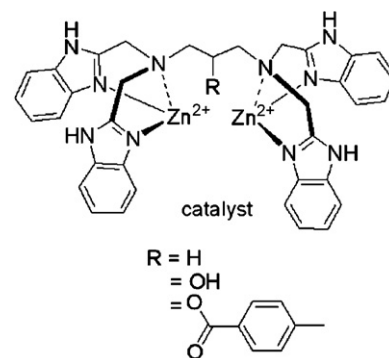


**Kortney L. Klinkel, Lauren A. Kiemele,  
Douglas L. Gin, John R. Hagadorn**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 173

Effect of ligand modifications and varying metal-to-ligand ratio on the catalyzed hydrolysis of phosphorus triesters by bimetallic tetrabenzimidazole complexes

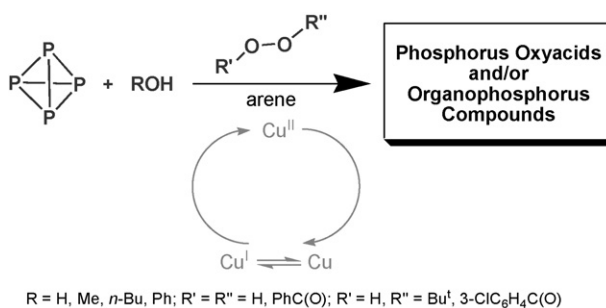
Systematic ligand modifications on certain elements of the binucleating tetrabenzimidazole ligand  $N,N,N',N'$ -tetrakis[(2-benzimidazolyl)methyl]-2-hydroxy-1,3-diaminopropane ( $^1L$ ) (i.e., certain functional groups, bridging linker length) and changes to the metal-to-ligand ratio were investigated as avenues for improving the catalytic performance of its dizinc(II) complex for the hydrolysis of the model phosphorus triester, *p*-nitrophenyl diphenyl phosphate (PNPDPP).



**Dina N. Akbayeva, Farida Kh. Faisova,  
Rumia R. Abdreimova, Maurizio Peruzzini**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 181

Oxidation of white phosphorus by peroxides in aqueous and alcoholic solutions: mechanistic aspects and catalytic studies

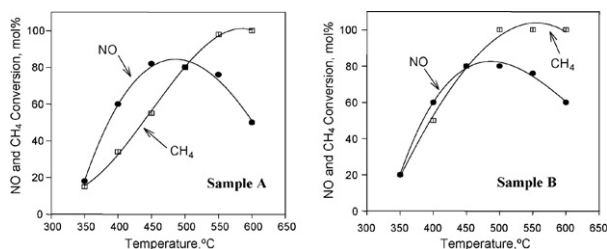


**Oscar A. Anunziata, Andrea R. Beltramone,  
Felix G. Requejo**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 194

In-containing BEA zeolite for selective catalytic reduction of  $\text{NO}_x$ . Part I: Synthesis, characterization and catalytic activity

In-HBEA prepared by ion exchange in liquid phase (IELP) using  $\text{InCl}_3$  (sample A) and In-HBEA prepared by ion exchange in solid phase (IESP) (sample B) are the most selective materials for the reduction of NO with methane; in this way methane is consumed selectively for the reduction of NO to  $\text{N}_2$  at 450–500 °C; this fact can be observed especially in the case of sample A.

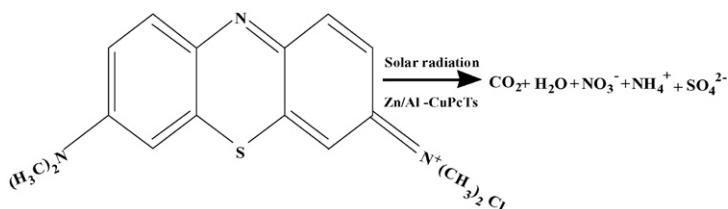


**K.M. Parida, N. Baliarsingh, B. Sairam Patra,  
J. Das**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 202

Copperphthalocyanine immobilized Zn/Al LDH as photocatalyst under solar radiation for decolorization of methylene blue

Zn/Al hydrotalcite-like compounds (HTLcs) with Zn/Al molar ratios of 2:1, 3:1, 4:1 were synthesized by co-precipitation method and were used as supports for the immobilization of Cu(II) tetrasulphonated phthalocyanine (CuPcTs). The photocatalytic decolorization of methylene blue (MB) was studied under solar radiation over Zn/Al (2:1)-(CuPcTs). The effect of time, pH, adsorbate concentration, catalyst dosage,  $\text{H}_2\text{O}_2$ , potassium persulphate and sodium chloride amount was studied as a function of the percentage of decolorization. The percentage of decolorization increases with the increase in pH of the solution. A maximum of 75% decolorization of methylene blue was achieved at 4 h solar irradiation.

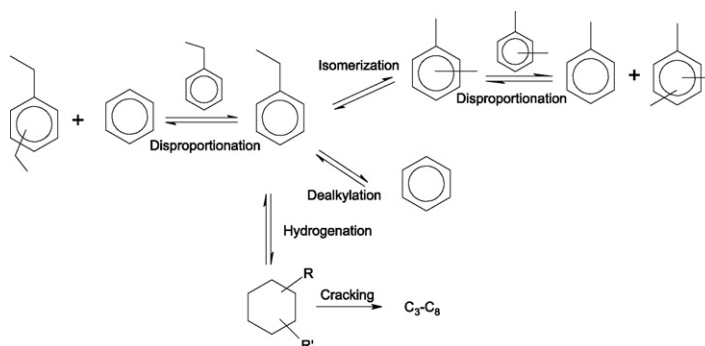


**A. Geetha Bhavani, A. Pandurangan**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 209

Hydroisomerization of ethylbenzene over bimetallic bifunctional zeolite catalysts

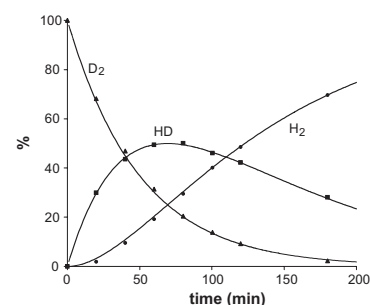
Enhancing the isomerization (xylene) selectivity with suppressing the side reactions by using Ni–Pt supported zeolites in vapour phase conditions.

**Jennifer L. Carriker, Paul S. Wagenknecht, Mitra A. Hosseini, Patrick E. Fleming**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 218

Transition metal catalyzed  $D_2/H_2O$  exchange: Distinguishing between the single and double exchange pathways

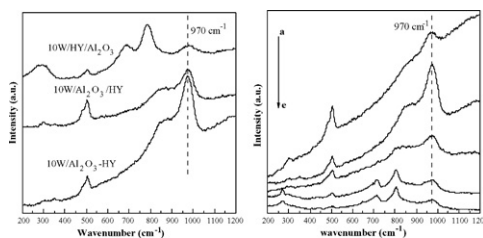
Rhodium complexes of water soluble phosphines catalyze H/D exchange between  $D_2$  and  $H_2O$ . This reaction has been monitored and the data have been fit to a model where either one or both atoms of  $D_2$  can exchange during one visit to the active site. The ratio of this single to double exchange varies with pH and mechanistic implications of this finding are discussed.

**Shengjun Huang, Fucun Chen, Shenglin Liu, Qingjun Zhu, Xiangxue Zhu, Wenjie Xin, Zaochi Feng, Can Li, Qingxia Wang, Longya Xu**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 224

The influence of preparation procedures and tungsten loading on the metathesis activity of ethene and 2-butene over supported  $WO_3$  catalysts

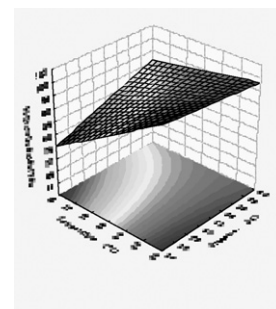
The correlation between the structure of supported tungsten oxide species and metathesis activities are investigated by UV Raman spectroscopy. Through the variation of preparation procedures and tungsten loadings, various tungsten species are co-present upon the  $Al_2O_3-HY$  support. The isolated tetrahedral tungsten oxide species are present on all active catalysts and should be the active sites precursors, which exhibit a characteristic Raman band at  $\sim 970\text{ cm}^{-1}$ .

**Andreia F. Peixoto, Mariette M. Pereira, Alberto A.C.C. Pais**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 234

Maximization of regioselectivity in hydroformylation of vinyl-aromatics using simple factorial design

A simple  $2^k$  factorial design has shown that a very significant increase in the regioselectivity of vinyl-aromatics (typically from 70% to more than 98%) can be obtained by the exclusive manipulation of two variables, pressure and temperature. It is also shown that optimised values can be obtained from within a range of possible values. The role of the ligand in the overall response of the system is also discussed and analysed.





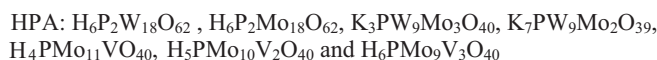
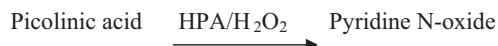
**Fateme F. Bamoharram, Majid M. Heravi, Mina Roshani, Fateme Abrishami**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 241

Catalytic N-oxidation of picolinic acid in the presence of heteropolyacids including Mo and W

The highly selective oxidation of picolinic acid with heteropoly anions including W and Mo in the presence of hydrogen peroxide give good to excellent yield of

the related N-oxides along with decarboxylation at 2- position of nitrogen.

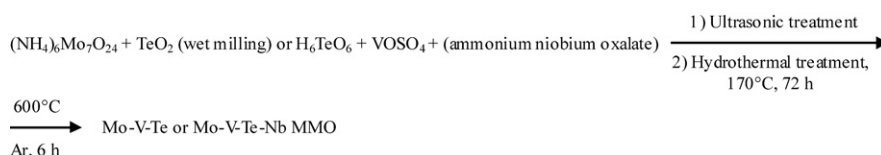


**Ru-Ming Feng, Xiu-Juan Yang, Wei-Jie Ji, Hai-Yang Zhu, Xiao-Dong Gu, Yi Chen, Scott Han, Hartmut Hibst**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 245

The study on the source of Te and the dispersion of  $\text{TeO}_2$  in fabricating Mo-V-Te and Mo-V-Te-Nb mixed metal oxide catalysts for propane partial oxidation

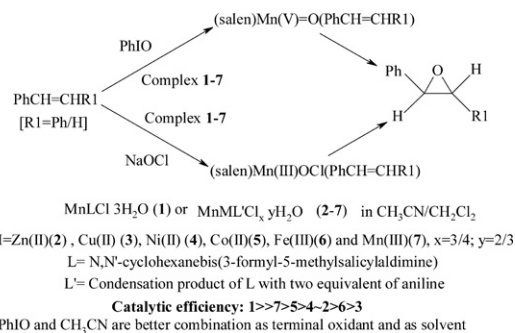
The effects of the source of Te and the dispersion of  $\text{TeO}_2$  on preparing Mo-V-Te and Mo-V-Te-Nb mixed metal oxide (MMO) catalysts have been systematically investigated. The employment of wet-milling and ultrasonic assisted dispersion of  $\text{TeO}_2$  was proved to be effective for making more active and selective Mo-V-Te/Mo-V-Te-Nb catalysts for propane partial oxidation.



**Tanmay Chattopadhyay, Samimul Islam, Munirathinam Nethaji, Adinath Majee, Debasis Das**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 255

Mono- and bi-metallic Mn(III) complexes of macroacyclic salen type ligands: Syntheses, characterization and studies of their catalytic activity

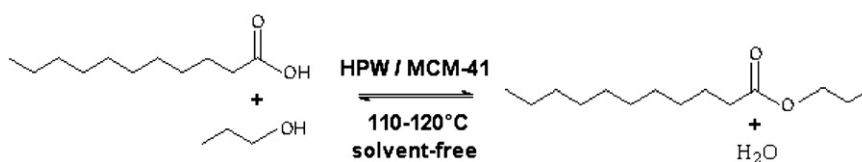


**Joon Ching Juan, Jingchang Zhang, Mohd Ambar Yarmo**

*Journal of Molecular Catalysis A: Chemical* 267 (2007) 265

12-Tungstophosphoric acid supported on MCM-41 for esterification of fatty acid under solvent-free condition

Supported HPW on MCM-41 were used as efficient solid acids for esterification of fatty acid under solventless conditions. The reaction mainly occurs inside the pores of MCM-41 because HPW loaded on as-synthesized catalyst shows lower conversion than calcined material.



**Oscar A. Anunziata, Andrea R. Beltramone,  
Eduardo J. Lede, Felix G. Requejo**

*Journal of Molecular Catalysis A: Chemical* 267  
(2007) 272

In-containing BEA zeolite for selective catalytic  
reduction of  $\text{NO}_x$ . Part II. Relation between In active  
sites and catalytic activity

For In-HBEA prepared by ion exchange in solid phase (Sample C) with higher Bronsted content, methane conversion increases, but the NO conversion is constant or decreases. Methane is not consumed to reduce NO. In-HBEA prepared by ion exchange in liquid phase using  $\text{InCl}_3$  (Sample A) possess more  $\text{NO}_2^-$  adspecies and less Brönsted sites and these sites are capable to convert methane selectively to reduce NO to  $\text{N}_2$ . The In species in Sample A is  $\text{InO}^+$  by PAC characterization.

