

## Contents

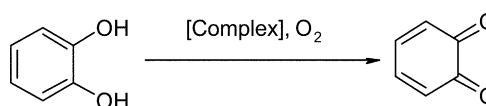
### Articles

**Davar M. Boghaei, Mahdi Behzad, Abolfazl Bezaatpour**

*Journal of Molecular Catalysis A: Chemical 241 (2005) 1*

Synthesis, characterization, electrochemical studies and catecholase-like activity of a series of mononuclear Cu(II), homodinuclear Cu(II)Cu(II) and heterodinuclear Cu(II)Ni(II) complexes of a phenol-based compartmental ligand

The initial rate of the oxidation of catechol to corresponding quinone was examined in the presence of a series of novel or previously reported mononuclear Cu(II), homodinuclear Cu(II)Cu(II) and heterodinuclear Cu(II)Ni(II) complexes. It is found that the homodinuclear complexes are more effective catalyst compared to the other complexes.

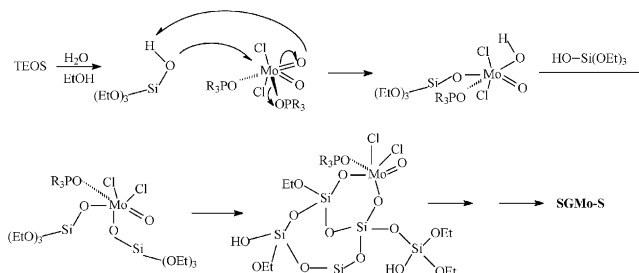


**Ge Wang, Linsheng Feng, Rudy L. Luck, David G. Evans, Zhiqiang Wang, Xue Duan**

*Journal of Molecular Catalysis A: Chemical 241 (2005) 8*

Sol–gel synthesis, characterization and catalytic property of silicas modified with oxomolybdenum complexes

Active solid oxidation catalysts can be obtained by incorporating dioxomolybdenum(VI) species derived from MoO<sub>2</sub>Cl<sub>2</sub>(OPMePh<sub>2</sub>)<sub>2</sub> into silica matrices via a sol–gel method, and can catalyze epoxidation. The supported catalyst has been characterized by elemental analysis, XRD, N<sub>2</sub>-physisorption, FT-IR, FT-Raman, UV–vis and solid-state MAS NMR spectroscopies, and a pathway for the reaction between MoO<sub>2</sub>Cl<sub>2</sub>(OPMePh<sub>2</sub>)<sub>2</sub> and tetraethoxysilane (TEOS) is suggested.

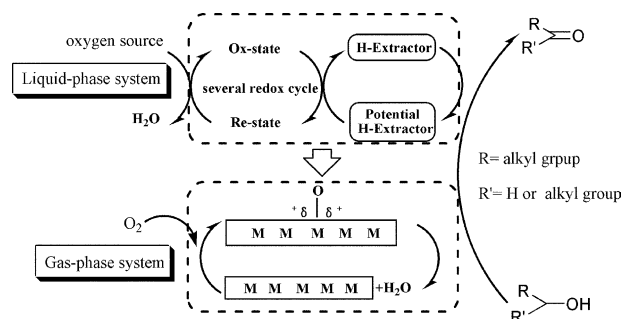


**Zhi Yang, Jing Li, Xiangguang Yang, Xiaofan Xie, Yue Wu**

*Journal of Molecular Catalysis A: Chemical 241 (2005) 15*

Gas-phase oxidation of alcohols over silver: The extension of catalytic cycles of oxidation of alcohols in liquid-phase

The oxidation of alcohols over silver is described. And the oxygen species play versatile roles in the above processes: basic sites and oxidative sites. The facets of silver integrate the several active catalytic sites existing in liquid-phase catalytic oxidation of alcohols.

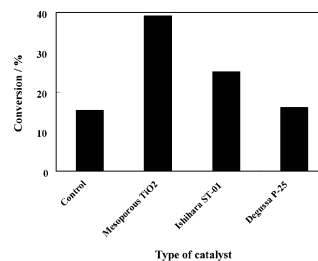
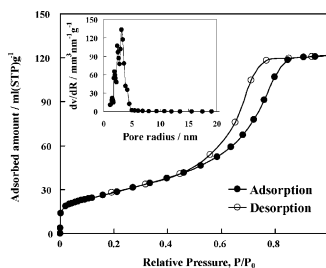


**Thammanoon Sreethawong, Yusuke Yamada, Tetsuhiko Kobayashi, Susumu Yoshikawa**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 23

Catalysis of nanocrystalline mesoporous TiO<sub>2</sub> on cyclohexene epoxidation with H<sub>2</sub>O<sub>2</sub>: Effects of mesoporosity and metal oxide additives

Nanocrystalline mesoporous TiO<sub>2</sub> with narrow and monomodal pore size distribution prepared by surfactant-assisted templating sol-gel process of laurylamine hydrochloride/tetraisopropyl orthotitanate modified with acetylacetone system exhibits higher catalytic cyclohexene epoxidation activity than non-mesoporous commercial TiO<sub>2</sub> powders.

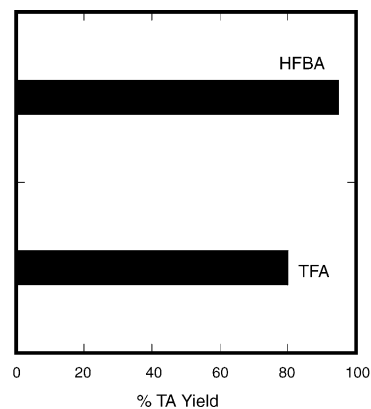


**Basudeb Saha, James H. Espenson**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 33

Combined acid additives and the MC catalyst for the autoxidation of *p*-xylene to terephthalic acid

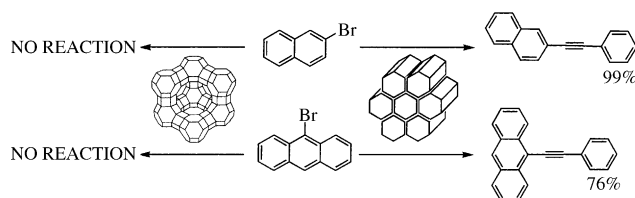
The autoxidation of *p*-xylene was carried out with the Co(OAc)<sub>2</sub>/Mn(OAc)<sub>2</sub>/Br<sup>-</sup> catalyst in the presence of acid additives, such as trifluoroacetic acid (TFA), heptafluorobutyric acid (HFBA) and *p*-toluenesulfonic acid. All the acid additives at low concentrations significantly improved the effectiveness of the catalyst. Under comparable reaction conditions and time, HFBA gave a 15% higher yield of terephthalic acid than TFA.



**Patrick Rollet, Wolfgang Kleist, Véronique Dufaud, Laurent Djakovitch**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 39

Copper-free heterogeneous catalysts for the Sonogashira cross-coupling reaction: Preparation, characterisation, activity and applications for organic synthesis



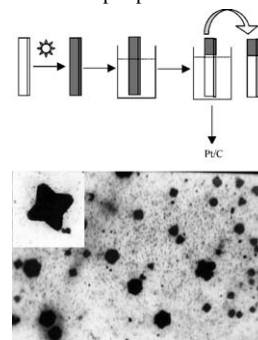
**S. Shanmugam, B. Viswanathan, T.K. Varadarajan**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 52

Preparation of noble metal supported carbon electrodes using photochemically reduced heteropolyanions in composite films

A novel reduction technique is developed for preparing a Pt/C system using organic-inorganic nanocomposite consisting of heteropolyanions. Transmission electron microscopic studies revealed the formation of anisotropic platinum nanocrystals. Cyclic voltammetry and electrochemical impedance spectroscopy were employed to evaluate the electrochemical methanol oxidation over the prepared Pt/C electrode. The obtained Pt/C catalysts were found to exhibit higher activity and stability for methanol oxidation in perchloric acid than in sulphuric acid medium. The activation energy for methanol oxidation was found to be 41±3kJmol<sup>-1</sup>, being lower than the reported value. The lower activation energy for methanol

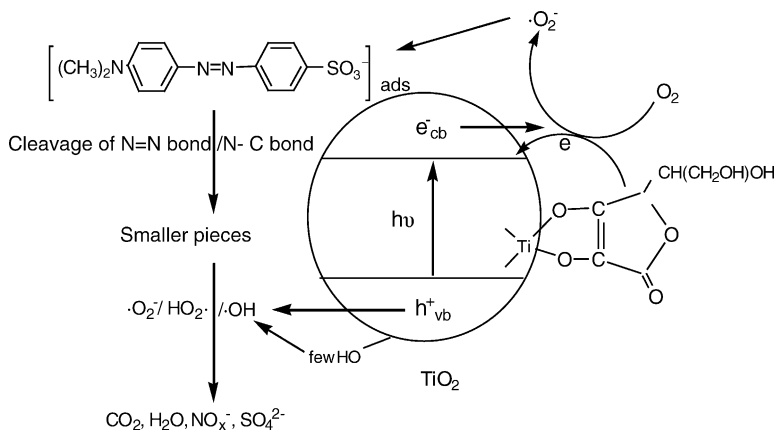
oxidation on Pt/C could be attributed to the presence of anisotropic platinum nanoparticles.



**Yan Ou, Jing-Dong Lin, Hong-Mei Zou,  
Dai-Wei Liao**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 59

Effects of surface modification of TiO<sub>2</sub> with ascorbic acid on photocatalytic decolorization of an azo dye reactions and mechanisms

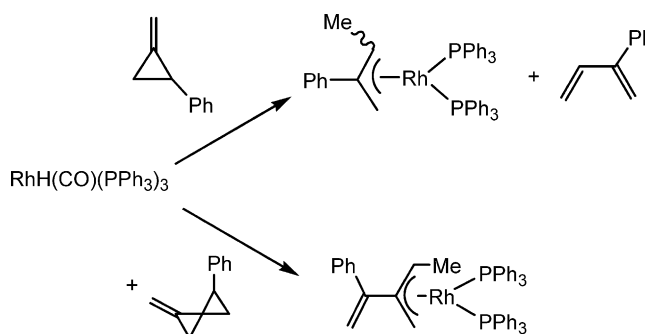


**Masumi Itazaki, Yasushi Nishihara,  
Hisami Takimoto, Chikako Yoda,  
Kohtaro Osakada**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 65

Ring-opening isomerization of methylenecyclopropanes catalyzed by hydridorhodium(I) complexes

RhH(CO)(PPh<sub>3</sub>)<sub>3</sub> promotes ring-opening isomerization of 2-phenyl-1-methylenecyclopropane and 4-phenyl-1-methylenespiro[2.2]pentane.

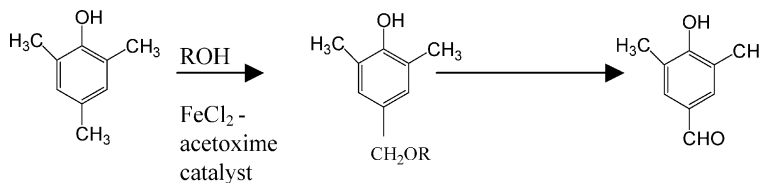


**Kuo-Tseng Li, Pang-Yih Liu**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 72

2,4,6-Trimethylphenol oxidation with ferrous chloride catalyst: Effect of acetoxime addition

Selective oxidation of 2,4,6-trimethylphenol to 3,5-dimethyl-4-hydroxybenzaldehyde with a FeCl<sub>2</sub>-acetoxime catalyst system is reported. The addition of acetoxime significantly increased the activity and selectivity. A reaction mechanism was employed successfully to explain the experimental results obtained. The activity improvement with the addition of acetoxime was ascribed to its better electron-donating ability, which enhanced the dissociation rate of the intermediate complex.

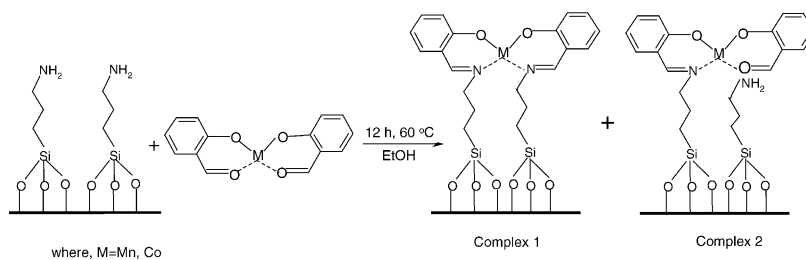


**V.D. Chaube, S. Shylesh, A.P. Singh**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 79

Synthesis, characterization and catalytic activity of Mn(III)- and Co(II)-salen complexes immobilized mesoporous alumina

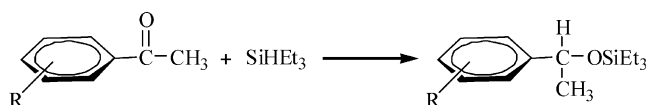
Mn(III)- and Co(II)-salen complexes immobilized mesoporous alumina were synthesized through the reaction of mesoporous alumina functionalized 3-aminopropyl triethoxy silane (3-APTES) and salicylic aldehyde via schiff base condensation.



**Murat Yiğit, Ismail Özdemir, Bekir Çetinkaya, Engin Çetinkaya**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 88

Novel *N*-heterocyclic-carbene–rhodium complexes as hydrosilylation catalysts

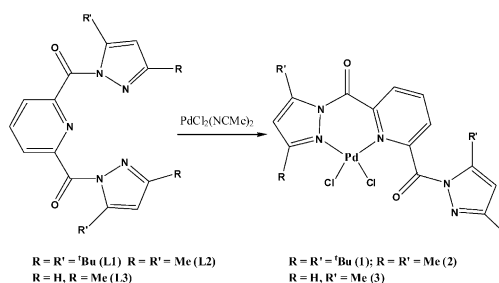


**M. Sarah Mohlala, Ilia A. Guzei, James Darkwa, Selwyn F. Mapolie**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 93

Pyridine linker pyrazolyl palladium complexes: Synthesis, characterization and ethylene polymerization activity

The reactions of bis(substituted-pyrazolylcarbonyl)pyridine compounds with  $[\text{PdCl}_2(\text{NCMe})_2]$  produce catalyst precursors for ethylene polymerization, in which one of the pyrazolyl units does not coordinate to the palladium. When these precursors were activated with methylaluminoxane (MAO) they catalyzed the polymerization of ethylene to linear high-density polyethylene.

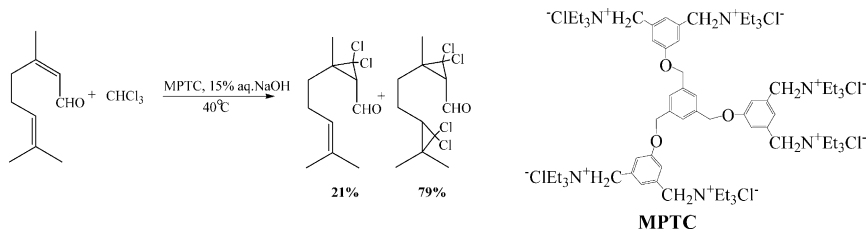


**Ayyanar Siva, Eagambaram Murugan**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 101

Synthesis and characterization of novel multi-site phase transfer catalyst and its catalytic efficiency for dichlorocarbene addition to citral

Novel soluble “multi-site (6 site)” phase transfer catalyst viz., 1,3,5-tris[4-(2,3-bis(triethylammonium-methylene chloride))-phenoxy]methyl]benzene (TEAMCPB) has been prepared by a simplified method and thoroughly characterized. It is shown to be  $\cong 10$ -fold higher effective than the commercially available single-site PTCs in catalysing the dichlorocarbene addition to citral under identical reaction conditions.

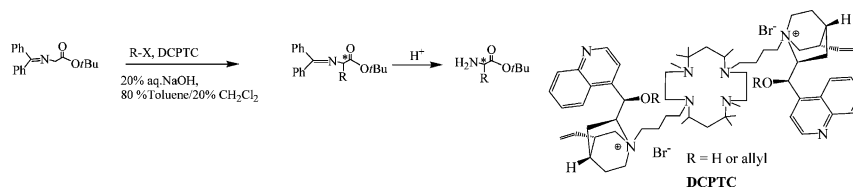


**Ayyanar Siva, Eagambaram Murugan**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 111

Syntheses of new dimeric-Cinchona alkaloid as a chiral phase transfer catalysts for the alkylation of Schiff base

New dimeric cinchona salts were synthesized and used as efficient chiral phase transfer catalysts for the synthesis of enantioselective alkylation of *N*-(diphenylmethylene)glycine *tert*-butyl ester giving very good chemical yield and ees.

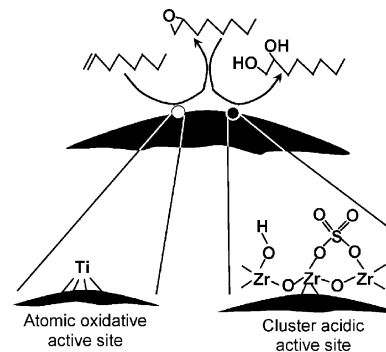


**Didik Prasetyoko, Zainab Ramli,  
Salasiah Endud, Hadi Nur**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 118

TS-1 loaded with sulfated zirconia as bifunctional oxidative and acidic catalyst for transformation of 1-octene to 1,2-octanediol

The consecutive transformation of 1-octene to 1,2-octanediol through the formation of 1,2-epoxyoctane using aqueous hydrogen peroxide has been carried out over bifunctional oxidative and acidic catalysts. The catalysts have been prepared by dispersion of sulfated zirconia on the TS-1.

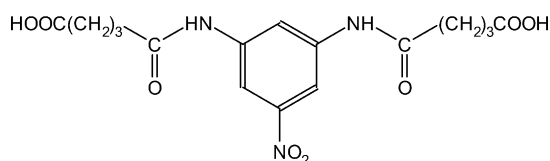


**Jasna Malešič, Matija Strlič, Jana Kolar,  
Slovenko Polanc**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 126

The influence of halide and pseudo-halide antioxidants in Fenton-like reaction systems containing copper(II) ions

Evaluation of the rate of oxidising species generation in Fenton-like systems containing copper(II) ions in the presence of halide and pseudo-halide antioxidants employing the *N,N'*-(5-nitro-1,3-phenylene)bis-glutaramide (NPG) hydroxylation assay.

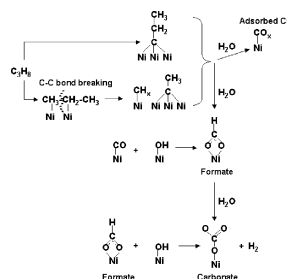


**Sittichai Natesakhawat, Okan Oktar,  
Umit S. Ozkan**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 133

Effect of lanthanide promotion on catalytic performance of sol-gel Ni/Al<sub>2</sub>O<sub>3</sub> catalysts in steam reforming of propane

The effect of lanthanide elements (La, Ce, and Yb) on the catalytic behavior of sol-gel Ni/Al<sub>2</sub>O<sub>3</sub> catalysts in propane steam reforming was investigated. The changes in reaction performance are related to catalyst reducibility, nickel surface area and resistance to deactivation. In situ DRIFTS results reveal mechanistic transformations after propane adsorption and subsequent reaction with water.

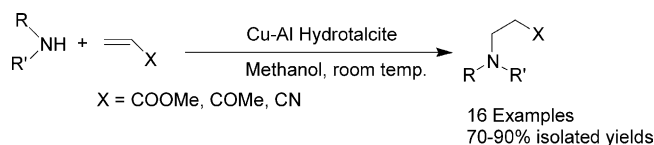


**M. Lakshmi Kantam, B. Neelima,  
Ch. Venkat Reddy**

*Journal of Molecular Catalysis A: Chemical* 241 (2005) 147

A recyclable protocol for aza-Michael addition of amines to  $\alpha,\beta$ -unsaturated compounds using Cu-Al hydrotalcite

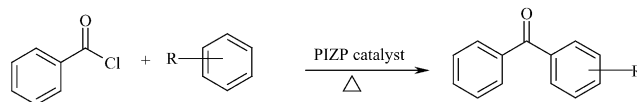
A recyclable protocol for aza-Michael addition of amines to  $\alpha,\beta$ -unsaturated compounds using Cu-Al hydrotalcite Aza-Michael adducts are obtained in very good yields by the conjugate addition of amines to  $\alpha,\beta$ -unsaturated compounds using Cu-Al-CO<sub>3</sub> hydrotalcite catalyst. The catalyst is used for four cycles with consistent activity and selectivity.



**M.B. Gawande, S.S. Deshpande,  
S.U. Sonavane, R.V. Jayaram**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 151

A novel sol-gel synthesized catalyst for Friedel-Crafts benzylation reaction under solvent-free conditions



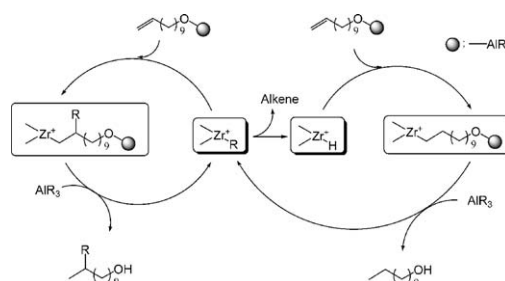
R = -H, -CH<sub>3</sub>, 1, 2 - (CH<sub>3</sub>)<sub>2</sub>, 1, 4 - (CH<sub>3</sub>)<sub>2</sub>, 1, 3, 5 - (CH<sub>3</sub>)<sub>3</sub>, -OCH<sub>3</sub>, -Cl, -Br

**Nobuo Kawahara, Shin-ichi Kojoh,  
Shingo Matsuo, Hideyuki Kaneko,  
Tomoaki Matsugi, Norio Kashiwa**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 156

Investigation of insertion reaction of 10-undecen-1-ol protected with alkylaluminum in En(Ind)<sub>2</sub>ZrCl<sub>2</sub>/MAO catalyst system

Insertion reaction of 10-undecen-1-ol protected with trialkylaluminums into the metallocene active center of En(Ind)<sub>2</sub>ZrCl<sub>2</sub>/MAO was confirmed in the absence of olefin monomers by GC and NMR analyses. It could be concluded that the insertion reaction of 10-undecen-1-ol occurred catalytically accompanied with an alkyl exchange reaction.

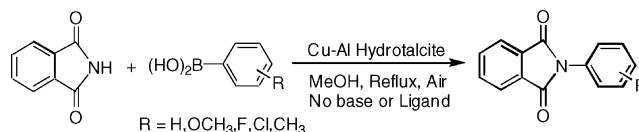


**M. Lakshmi Kantam, B. Veda Prakash,  
Ch. Venkat Reddy**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 162

N-arylation of imides with arylboronic acids using Cu-Al hydrotalcite

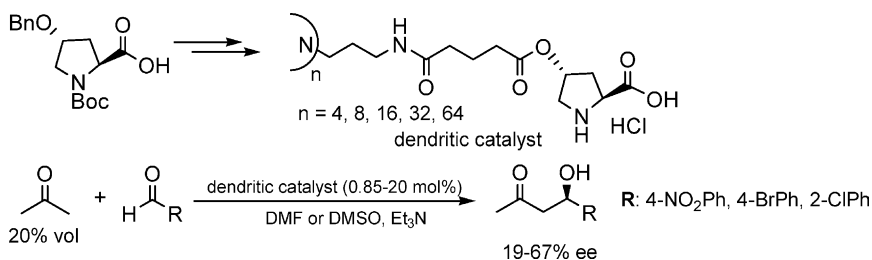
Arylation of imides with various boronic acids was performed using Cu-Al hydrotalcite in very good yields in refluxing methanol. The catalyst is used for four times successfully.



**Evangelos Bellis, George Kokotos**

*Journal of Molecular Catalysis A: Chemical* 241  
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Proline-modified poly(propyleneimine) dendrimers as catalysts for asymmetric aldol reactions

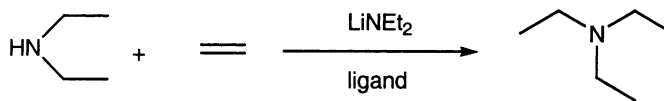


**Vivek Khedkar, Annegret Tillack,  
Christoph Benisch, Johann-Peter Melder,  
Matthias Beller**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 175

Base-catalyzed hydroamination of ethylene with diethylamine

The catalytic hydroamination reaction of ethylene with diethylamine in the presence of lithium diethylamide has been reinvestigated to improve catalyst productivity. Various tertiary amines were synthesized and screened as ligands for the target reaction.

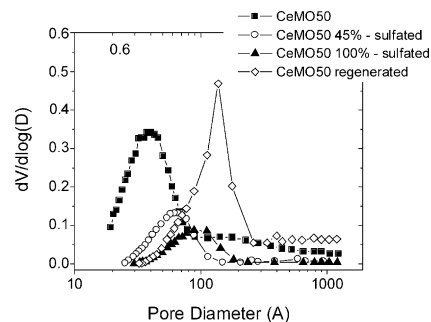


**Carla Maria Salerno Polato,  
Cristiane Assumpção Henriques,  
Arnaldo Alcover Neto,  
José Luiz Fontes Monteiro**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 184

Synthesis, characterization and evaluation of CeO<sub>2</sub>/Mg,Al-mixed oxides as catalysts for SO<sub>x</sub> removal

CeO<sub>2</sub>/Mg,Al-mixed oxide with Mg/Al=1, for which both an Mg(Al)O periclase-type and an MgAl<sub>2</sub>O<sub>4</sub>-spinel were present showed the best performance for SO<sub>x</sub> removal under conditions similar to those of FCC units. The sulfates formed from the spinel-phase are more easily reduced than those from the periclase phase. The growth of the sulfate phase in the early stages of sulfation destroys the small mesopores of the catalyst. Upon regeneration, the sulfate phase is consumed and larger mesopores are formed.



**Zhongkui Zhao, Weihong Qiao, Xiuna Wang,  
Guiru Wang, Zongshi Li, Lübo Cheng**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 194

HY zeolite promoted free-solvent alkylation of  $\alpha$ -methyl-naphthalene with long chain olefins in liquid–solid intermittent reaction

HY zeolite promoted liquid–solid free-solvent alkylations of  $\alpha$ -methyl-naphthalene with long chain olefins (mixed olefins,  $m+n=7$  and 8, mass ratio of C<sub>11</sub>:C<sub>12</sub> is 45:55) have been performed in intermittent reactor. The various reaction parameters are optimized. The HY zeolite could be a practical catalyst for long chain alkylation of  $\alpha$ -methyl-naphthalene.

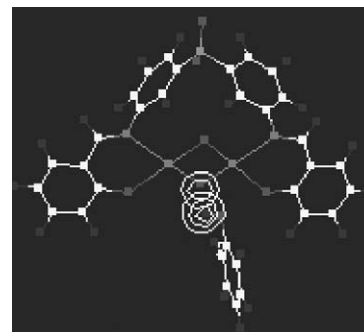


**Akinobu Shiga, Yasuhiko Kurusu**

*Journal of Molecular Catalysis A: Chemical* 241  
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Theoretical study on reaction between bis( $\mu$ -peroxo)dicopper(2)complex and phenol by “paired interacting orbitals (PIO)” analysis

A reaction between  $\mu$ - $\eta^2$ : $\eta^2$ -bridging peroxodicycopper complex of bis[3-(2-hydroxybenzylideneamino)phenyl]sulfone and phenol are investigated by using paired interacting orbitals (PIO) analysis proposed by Fujimoto et al. By observing the contour maps and overlap populations of main PIOs, it is clearly suggested that formation of mono-phenoxo complex is easy, however di-phenoxo complex formation is difficult.

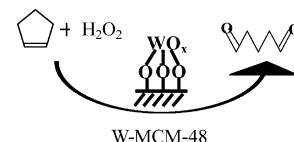


**Xin-Li Yang, Wei-Lin Dai, Ruihua Gao,  
Hui Chen, Hexing Li, Yong Cao, Kangnian Fan**

*Journal of Molecular Catalysis A: Chemical* 241  
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Synthesis, characterization and catalytic application of mesoporous W-MCM-48 for the selective oxidation of cyclopentene to glutaraldehyde

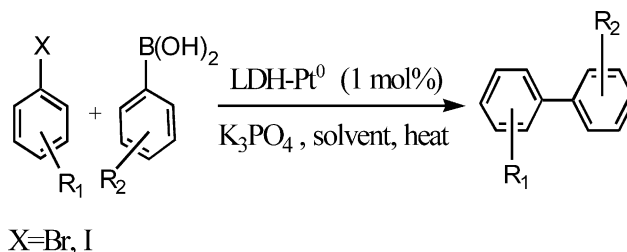
Tungsten-containing ordered MCM-48 has been synthesized under hydrothermal conditions via pH adjustment and was characterized with various analytical and spectroscopic techniques. The as-synthesized W-MCM-48 material is active as a heterogeneous catalyst for the selective oxidation of cyclopentene (CPE) to glutaraldehyde (GA) with environmentally benign aqueous hydrogen peroxide as the oxidant.



**Boyapati M. Choudary, Moumita Roy,  
Sarabindu Roy, M. Lakshmi Kantam**

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 215

Layered double hydroxides supported nanoplatinum catalyst for Suzuki coupling of aryl halides

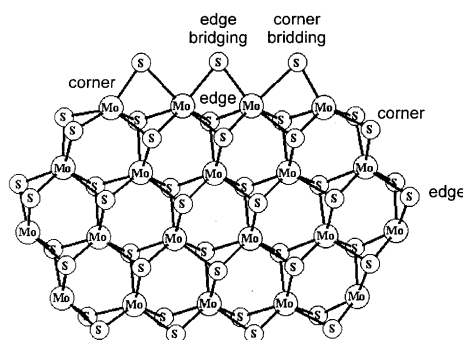


**Tao Zeng, Xiao-Dong Wen, Yong-Wang Li,  
Haijun Jiao**

*Journal of Molecular Catalysis A: Chemical* 241  
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Removal of surface sulfur from MoS<sub>x</sub> cluster under CO adsorption

The difference of the corner and edge sites in the removal of surface sulfur and CO adsorption.

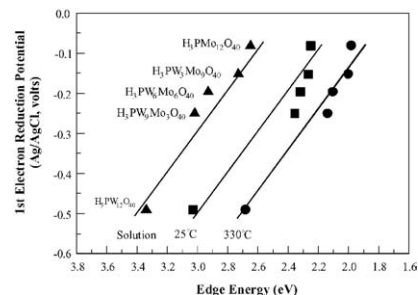


**Min Hye Youn, Heesoo Kim, Ji Chul Jung,  
In Kyu Song, Katherine P. Barteau,  
Mark A. Barteau**

*Journal of Molecular Catalysis A: Chemical* 241  
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UV-vis spectroscopy studies of H<sub>3</sub>PMo<sub>12-x</sub>W<sub>x</sub>O<sub>40</sub> heteropolyacid (HPA) catalysts in the solid state: Effects of water content and polyatom substitution

UV-vis spectroscopy studies of solid state H<sub>3</sub>PMo<sub>12-x</sub>W<sub>x</sub>O<sub>40</sub> (x=0, 3, 6, 9, 12) catalysts were carried out. The solid HPA catalysts were treated at 25 °C (squares) and 330 °C (circles). The absorption edge energies of the H<sub>3</sub>PMo<sub>12-x</sub>W<sub>x</sub>O<sub>40</sub> catalysts could be directly correlated with the reduction potentials of the HPA catalysts. The lower absorption edge energy corresponded to the higher reduction potential of the HPA catalyst.

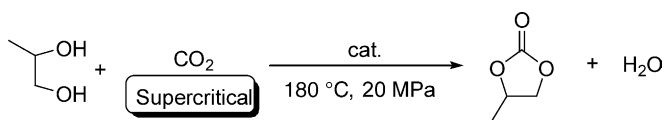




Ya Du, De-Lin Kong, Hai-Ying Wang, Fei Cai,  
Jie-Sheng Tian, Jin-Quan Wang,  
Liang-Nian He

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 233

Sn-catalyzed synthesis of propylene carbonate  
from propylene glycol and CO<sub>2</sub> under supercritical  
conditions



Jiquan Zhao, Yuecheng Zhang, Jianping Han,  
Yongjie Jiao

*Journal of Molecular Catalysis A: Chemical* 241  
(2005) 238

Preparation and performance of anchored hetero-  
genized rhodium complex catalyst for hydrofor-  
mylation

The immobilized catalyst for hydroformylation was prepared and characterized by FT-IR, X-ray photoelectron spectroscopy (XPS), TG-DTA, ICP and N<sub>2</sub> absorption. The performance of the catalyst in the hydroformylation of 1-hexene was studied.

