

## Contents

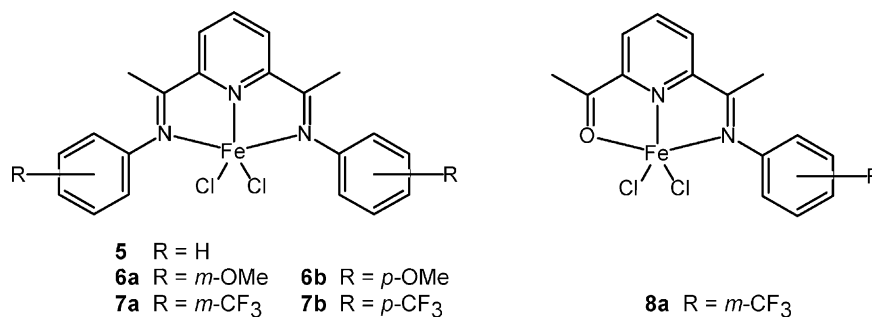
### Articles

**Martin E. Bluhm, Cristina Folli,  
Manfred Döring**

*Journal of Molecular Catalysis A: Chemical 212  
(2004) 13*

New iron-based bis(imino)pyridine and acetyl-  
imino-pyridine complexes as single-site catalysts for  
the oligomerization of ethylene

New iron-based bis(imino)pyridine complexes **6**, **7** and the acetyl-imino-pyridine complex **8a** are active catalysts together with the co-catalyst MAO for the oligomerization of ethylene. The influence of electron donating methoxy- and electron withdrawing trifluoromethyl-groups attached to the imino phenyl substituents is tested in the catalysis.

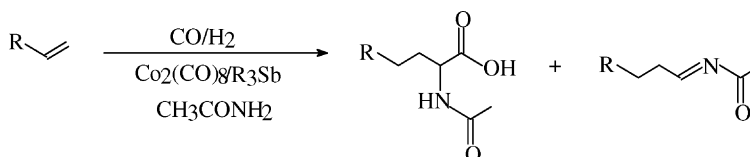


**Armando Cabrera, Pankaj Sharma,  
José Luis Arias, José Luis Velasco,  
Javier Pérez-Flores, Rosa María Gómez**

*Journal of Molecular Catalysis A: Chemical 212  
(2004) 19*

Amidocarbonylation of alkenes at very low pres-  
sures with a Co<sub>2</sub>(CO)<sub>8</sub>/SbR<sub>3</sub> system: two easy  
routes to reach *N*-acetyl- $\alpha$ -aminoacids

Amidocarbonylation reaction catalysed by a Co<sub>2</sub>(CO)<sub>8</sub>/SbR<sub>3</sub> system was carried out to obtain *N*-acetyl- $\alpha$ -aminoacids from several alkenes. The use of R<sub>3</sub>Sb ligands not only enhances the catalytic activity but also increases the selectivity at very low pressures.

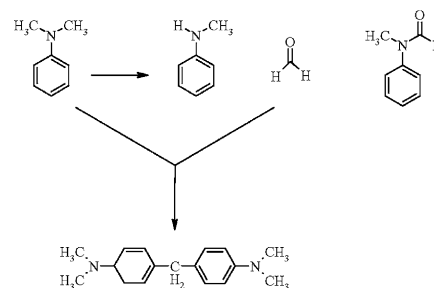


**Dorota Naróg, Urszula Lechowicz,  
Tadeusz Pietryga, Andrzej Sobkowiak**

*Journal of Molecular Catalysis A: Chemical 212  
(2004) 25*

Iron(II, III)-catalyzed oxidative *N*-dealkylation of  
amines with dioxygen

Labile iron complexes in base-free acetonitrile activate dioxygen for the direct oxygenation of *N,N*- and *N*-alkylated amines to form *N*-dealkylated products and corresponding aldehydes. Iron(III) catalysts are rapidly reduced by the substrate to iron(II), which activates dioxygen. Dioxygen activation step is preceded by the equilibrium reaction between iron(II) catalyst and substrate.

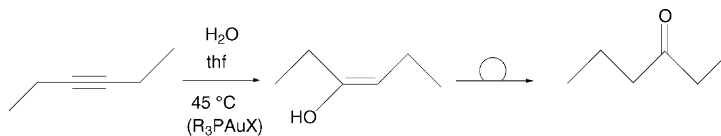


**Patric Roembke, Hubert Schmidbaur,  
Stephanie Cronje, Helgard Raubenheimer**

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 35

Application of (phosphine)gold(I) carboxylates, sulfonates and related compounds as highly efficient catalysts for the hydration of alkynes

A series of six gold(I) complexes LAuX (L = Ph<sub>3</sub>P, X = CO<sub>2</sub>C<sub>2</sub>F<sub>5</sub>, SO<sub>3</sub>-*p*-tol, SO<sub>3</sub>Et, SSO<sub>2</sub>-*p*-tol; L = Me<sub>3</sub>P, (*p*-tol)<sub>3</sub>P, X = CO<sub>2</sub>C<sub>2</sub>F<sub>5</sub>) have been used as highly active catalysts for the hydration of 3-hexyne forming 3-hexanone in the presence of BF<sub>3</sub>·Et<sub>2</sub>O as a co-catalyst. Similar silver(I) complexes have also been investigated in this regard and an explanation for their lack of activity is given in this paper.



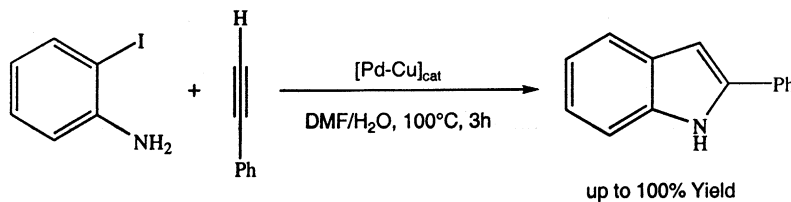
R = Ph, Me, *p*-Tol

X = OC(O)C<sub>2</sub>F<sub>5</sub>, OS(O)<sub>2</sub>-*p*-tol, OS(O)<sub>2</sub>Et, SS(O)<sub>2</sub>-*p*-tol

**Sandra Chouzier, Markus Gruber,  
Laurent Djakovitch**

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 43

New hetero-bimetallic Pd-Cu catalysts for the one-pot indole synthesis via the Sonogashira reaction

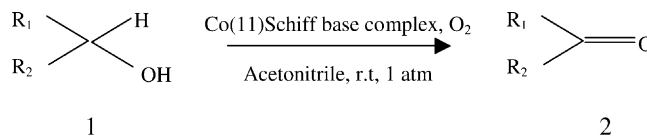


**Vishal B. Sharma, Suman L. Jain, Bir Sain**

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 55

Cobalt (II) Schiff base catalyzed aerobic oxidation of secondary alcohols to ketones

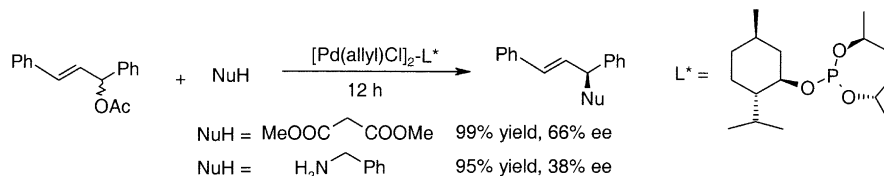
The oxidation of a variety of secondary alcohols to corresponding ketones with molecular oxygen using cobalt (II) Schiff base complexes as catalysts is reported.



**Jean Michel Brunel, Bruno Faure**

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 61

Enantioselective palladium catalyzed allylic substitution with a new phosphite ligand issued from (2*S*,5*S*)-hexanediol

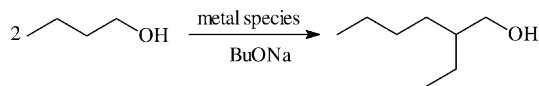


**Carlo Carlini, Alessandro Macinai,  
Anna Maria Raspolli Galletti, Glauco Sbrana**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 65

Selective synthesis of 2-ethyl-1-hexanol from *n*-butanol through the Guerbet reaction by using bifunctional catalysts based on copper or palladium precursors and sodium butoxide

The catalytic synthesis of 2-ethyl-1-hexanol, via the Guerbet self-condensation of *n*-butanol, has been studied. Bifunctional catalysts based on copper chromite as well as palladium derivatives as dehydrogenating/hydrogenating metal species and sodium butoxide (BuONa) as the basic component were investigated in dependence of the reaction parameters.

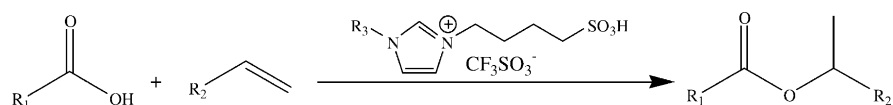


**Yanlong Gu, Feng Shi, Youquan Deng**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 71

Esterification of aliphatic acids with olefin promoted by Brønsted acidic ionic liquids

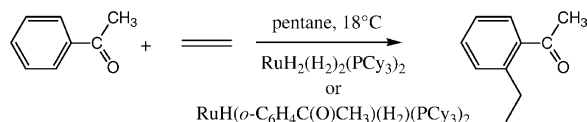
SO<sub>3</sub>H-functionalized ionic liquids could be an efficient catalyst for esterification of aliphatic acids with olefins. The produced esters could be easily separated by decantation and the ionic liquids as catalyst could be reused.



**Yannick Guari, Aida Castellanos,  
Sylviane Sabo-Etienne, Bruno Chaudret**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 77

RuH<sub>2</sub>(H<sub>2</sub>)<sub>2</sub>(PCy<sub>3</sub>)<sub>2</sub>: a room temperature catalyst for the Murai reaction

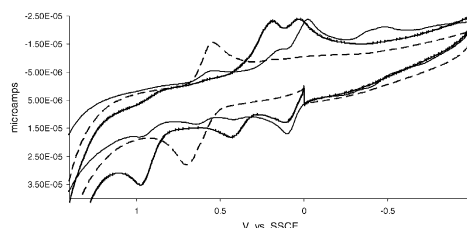


**Estelle L. Lebeau**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 83

Instability of the oxidation catalysts [Os<sup>III</sup>(tpy)(bpy)(py)]<sup>3+</sup> and [Os<sup>III</sup>(bpy)<sub>3</sub>]<sup>3+</sup> in alkaline solution

The Os(III) complexes [Os<sup>III</sup>(tpy)(bpy)(py)]<sup>3+</sup> and [Os<sup>III</sup>(bpy)<sub>3</sub>]<sup>3+</sup> (bpy: 2,2'-bipyridine, py: pyridine, tpy: 2,2',2''-terpyridine) are unstable toward self-reduction in alkaline solution. Product analysis performed by using UV-Vis spectroscopy, cyclic voltammetry, HPLC and GC show that ca. 90% of the reduced product that appears is the unmodified polypyridyl complex of Os(II), [Os<sup>II</sup>(tpy)(bpy)(py)]<sup>2+</sup> or [Os<sup>II</sup>(bpy)<sub>3</sub>]<sup>2+</sup>. Another product of the reduction of [Os<sup>III</sup>(tpy)(bpy)(py)]<sup>3+</sup> in basic solution has been identified as [Os<sup>II</sup>(tpy)(bpy)(OH<sub>2</sub>)]<sup>2+</sup> which results from metal reduction and concomitant pyridine ligand loss.

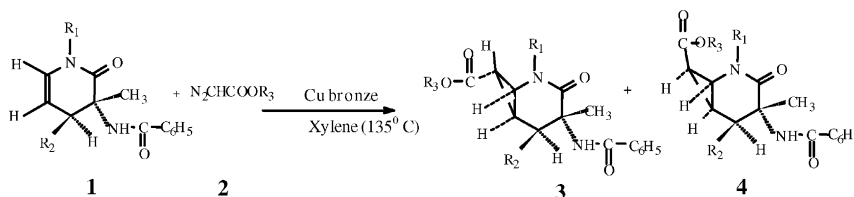


**Suman L. Jain, Bir Sain**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 91

Copper-catalyzed cyclopropanation of 1,2,3,4-tetrahydropyridin-2-ones with diazoacetates. A facile and stereoselective synthesis of 3-oxo-2-azabicyclo [4.1.0] heptanes

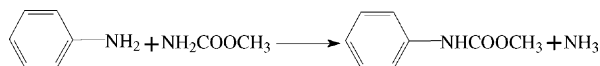
Reactions of a series of 1,2,3,4-tetrahydropyridin-2-ones (**1**) with diazoacetates (**2**) in presence of copper bronze catalyst to yield exclusively 3-oxo-2-aza-bicyclo [4.1.0] heptanes (**3** and **4**) in excellent yields with high *exo*-selectivity are reported.

**Qi-Feng Li, Jun-Wei Wang, Wen-Sheng Dong, Mao-Qing Kang, Xin-Kui Wang, Shao-Yi Peng**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 99

A phosgene-free process for the synthesis of methyl *N*-phenyl carbamate by the reaction of aniline with methyl carbamate

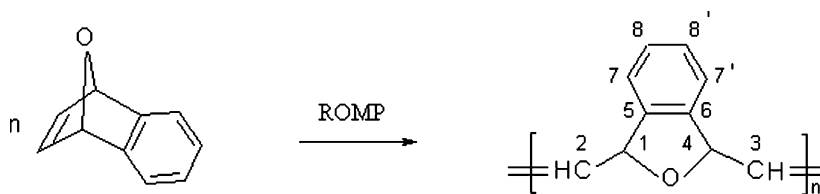
Methyl *N*-phenyl carbamate (MPC) was synthesized by the reaction of aniline with methyl carbamate in the presence of methanol over ZnCl<sub>2</sub> catalyst. Effects of catalysts, reaction temperature, reaction time, and catalyst content, the molar ratio of reactants and the content of water on the reaction were investigated. A possible reaction mechanism was proposed based on the product distribution.

**Valia Amir-Ebrahimi, John J. Rooney**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 107

The remarkable activity of 7-oxa-benzonorbornadiene in metathesis copolymerization using Ru-based initiators

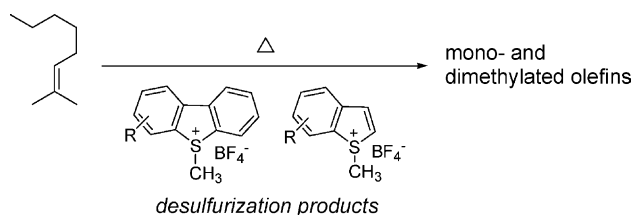
The remarkable reactivity of 7-oxa-benzonorbornadiene in olefin metathesis using Ru-based initiators is shown in studies of its copolymerization with benzonorbornadiene, norbornene and cyclopentene. The facilitating effect of the presence of the 7-oxygen atom on the [2 + 2] cyclobutane step is discussed.

**Yasuhiro Shiraishi, Takayuki Hirai**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 115

Transmethylation of olefin via *S*-methylsulfonium salts obtained by desulfurization of light oil

*S*-Methylsulfonium salts, obtained by a desulfurization process for light oil based on methylation of sulfur compounds using CH<sub>3</sub>I and AgBF<sub>4</sub>, were used as a methyl-transfer agent for transmethylation of 2-methyl-2-octene. The salts showed high transmethylation activity. This is because the salts are derived from highly alkyl-substituted dibenzothiophenes and benzothiophenes of low nucleophilicity and release the methyl group very easily against thermal stimulation.

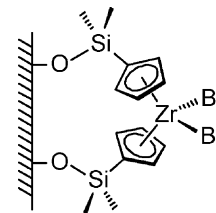


**Xu Cheng, Owen W. Lofthus, Paul A. Deck**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 121

Ethylene polymerization using silica-supported zirconocene dibromide/methylalumoxane catalysts

Electrophile-functionalized zirconocene dibromide catalysts were supported on silica and screened for ethylene polymerization activity in toluene solution using methylalumoxane (MAO) as cocatalyst. Supported catalysts showed moderate activity and stability toward leaching.

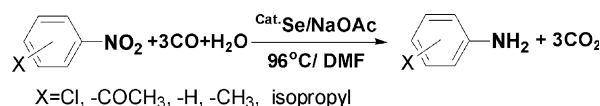


**Xiaozhi Liu, Shiwei Lu**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 127

Selective formation of aromatic amines by selenium-catalyzed reduction of aromatic nitro compounds with CO/H<sub>2</sub>O under atmospheric pressure

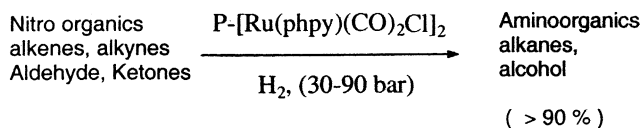
In the presence of selenium as a catalyst, the aromatic nitro compounds are quantitatively reduced by CO/H<sub>2</sub>O to form the corresponding amines under atmospheric pressure. The reduction occurs in high selectivity regardless of the substitution groups on the aromatic ring and without affecting other reducible functionality.



**S.M. Islam, C.R. Saha**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 131

Polystyrene anchored orthometalated ruthenium(II) complex as catalyst for the dihydrogen reduction of unsaturated organic substrates

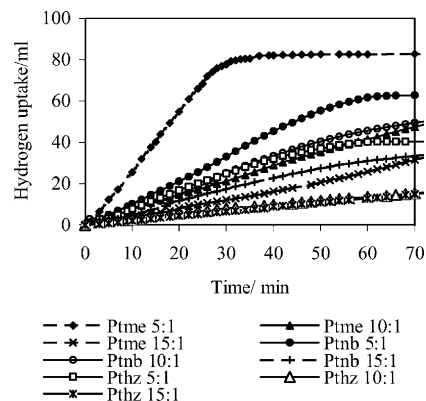


**M. Adlim, Mohamad Abu Bakar, Kong Yong Liew, Jamil Ismail**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 141

Synthesis of chitosan-stabilized platinum and palladium nanoparticles and their hydrogenation activity

Chitosan-stabilized Pt or Pd particles of size of 1–2nm, were synthesized using CH<sub>3</sub>OH or NaBH<sub>4</sub> as the reducing agents. Activity for the hydrogenation of octene and cyclooctene of Pt was much higher than Pd. Pd but not Pt, also catalyzed the isomerization of the double bond.

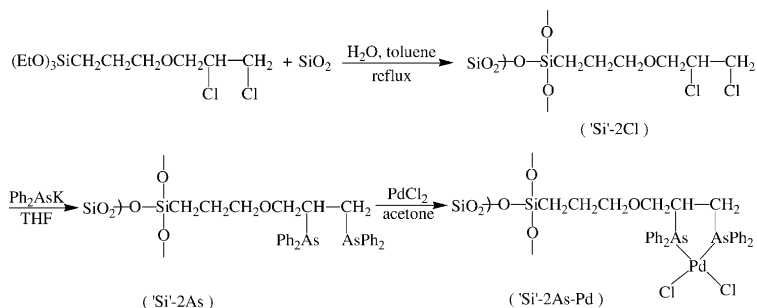


**Mingzhong Cai, Yizheng Huang, Ronghua Hu, Caisheng Song**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 151

Synthesis of silica-supported bidentate arsine palladium complex and its catalytic properties for amidation/butoxycarbonylation of aryl halides

The synthesis of a silica-supported bidentate arsine palladium complex has been described. This polymeric arsine palladium complex is an efficient catalyst for Heck carbonylation of aryl halides and can be recovered and reused.

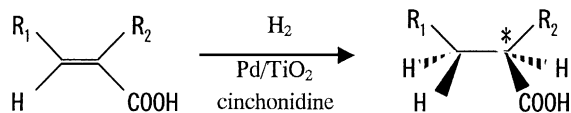


**Yuriko Nitta, Takeshi Kubota, Yasuaki Okamoto**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 155

Solvent effect on the structure sensitivity in enantioselective hydrogenation of  $\alpha,\beta$ -unsaturated acids with modified palladium catalysts

The structure sensitivity in the enantioselective hydrogenation of (*E*)-2,3-diphenyl-2-propenoic acid with cinchonidine-modified Pd/TiO<sub>2</sub> catalysts is solvent dependent, especially in the dispersion range lower than 0.2, while it is almost independent of the solvent polarity in the reactions of smaller aliphatic acids. The importance of the steric interference of the Pd surface with the modifier–substrate adduct is suggested.

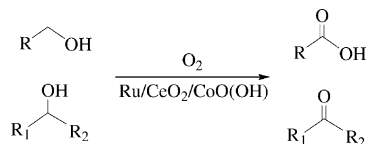


**Kohki Ebitani, Hong-Bing Ji, Tomoo Mizugaki, Kiyotomi Kaneda**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 161

Highly active trimetallic Ru/CeO<sub>2</sub>/CoO(OH) catalyst for oxidation of alcohols in the presence of molecular oxygen

The trimetallic Ru/CeO<sub>2</sub>/CoO(OH) compound acted as a highly efficient heterogeneous catalyst for the oxidation of various alcohols into the corresponding carbonyls, including less-reactive *primary* alcohols, in the presence of molecular oxygen under mild reaction conditions.

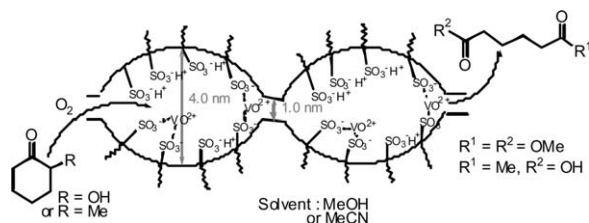


**Leïla El Aakel, Franck Launay, Jean-Marie Brégeault, Ahmed Atlamsani**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 171

Nafion<sup>®</sup>-supported vanadium oxidation catalysts: redox *versus* acid-catalysed ring opening of 2-substituted cycloalkanones by dioxygen

[VO]<sup>2+</sup>-Exchanged Nafion<sup>®</sup> catalysts are efficient in the aerobic C–C bond cleavage of 2-hydroxycyclohexanone and 2-methylcyclohexanone in methanol and acetonitrile, respectively. However, diffusion limitations, especially for the higher vanadyl contents have led to the design of different mixed redox and acid solid catalysts. The cleavage of  $\alpha$ -hydroxyketones can also be initiated by different Brønsted acids, including totally or partially protonated Nafion<sup>®</sup>.

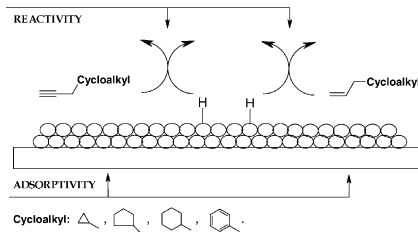


**Petr Kačer, Libor Červený**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 183

The influence of cycloalkylsubstituent on the hydrogenation of terminal alkyne and alkenic bonds on platinum and palladium catalysts

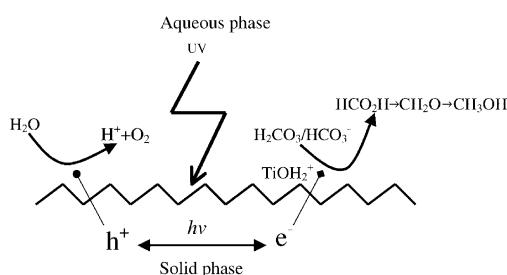
The work is concerned with structure effects exerted by molecules of substituted acetylenes and ethylenes (cyclopropyl, cyclopentyl, cyclohexyl, phenyl) in heterogeneously catalyzed hydrogenation on platinum and palladium supported catalysts. Kinetic parameters, acquired from hydrogenation of individual model substances as well as binary systems in competitive arrangements allowed the assessment of the relation between the molecular structure and the rate of a surface reaction in parallel with the stability of the surface complex

**Young Ku, Wan-Hui Lee, Wen-Yu Wang**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 191

Photocatalytic reduction of carbonate in aqueous solution by UV/TiO<sub>2</sub> process

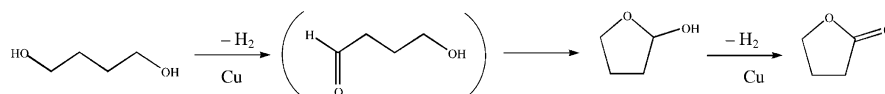
The temporal behavior of the photocatalytic reduction of carbonate in aqueous solution by the UV/TiO<sub>2</sub> process was studied under various solution pH values, TiO<sub>2</sub> dosage, and UV light intensities in order to determine the reaction rates. The reaction scheme is proposed below. A Langmuir–Hinshelwood type kinetic equation is developed for modeling the photocatalytic reduction of carbonate by the UV/TiO<sub>2</sub> process in aqueous solution.

**Naoki Ichikawa, Satoshi Sato, Ryoji Takahashi, Toshiaki Sodesawa, Kanichiro Inui**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 197

Dehydrogenative cyclization of 1,4-butanediol over copper-based catalyst

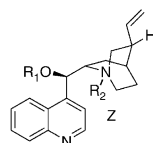
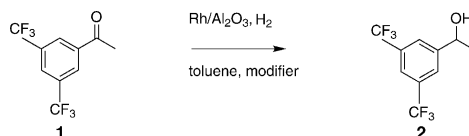
Synthesis of  $\gamma$ -butyrolactone (GBL) from 1,4-butanediol (BDO) over copper-based catalysts with ZnO, Al<sub>2</sub>O<sub>3</sub> and ZrO<sub>2</sub> was investigated. Catalytic activity of copper was greatly affected by the additive oxides. The highest activity was obtained at a catalyst molar ratio of CuO:ZnO:ZrO<sub>2</sub>:Al<sub>2</sub>O<sub>3</sub> = 6:1:2:2.

**Reto Hess, Frank Krumeich, Tamas Mallat, Alfons Baiker**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 205

Rhodium-catalyzed heterogeneous enantioselective hydrogenation of 3,5-di-(trifluoromethyl)-acetophenone

In the asymmetric hydrogenation of **1**, replacement of CD by its ether derivatives resulted in the inversion of enantioselectivity from (*S*)-**2** to (*R*)-**2**.



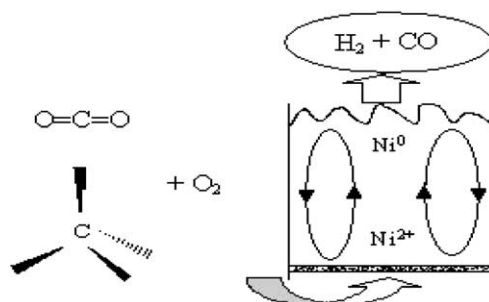
Modifier	R <sub>1</sub>	R <sub>2</sub>	Z
CD	H	-	-
MeOCD	methyl	-	-
EtOCD	ethyl	-	-
PhOCD	phenyl	-	-
TmsOCD	trimethylsilyl	-	-
CD•HCl	H	-	HCl
N-MeCDCI	H	methyl	Cl <sup>-</sup>
N-BzCDCI	H	benzyl	Cl <sup>-</sup>

**Qiangshan Jing, Hui Lou, Liuye Mo, Jinhua Fei, Xiaoming Zheng**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 211

Combination of CO<sub>2</sub> reforming and partial oxidation of methane over Ni/BaO-SiO<sub>2</sub> catalysts to produce low H<sub>2</sub>/CO ratio syngas using a fluidized bed reactor

Addition of BaO on Ni/SiO<sub>2</sub> might be responsible for its high activity and resistance to sintering because it can produce a highly dispersed active surface area as bound-state Ni species. The promoted 5Ni/SiO<sub>2</sub> catalysts were active and stable for combined CO<sub>2</sub> reforming and partial oxidation of methane to produce low H<sub>2</sub>/CO ratio syngas using a fluidized bed reactor.

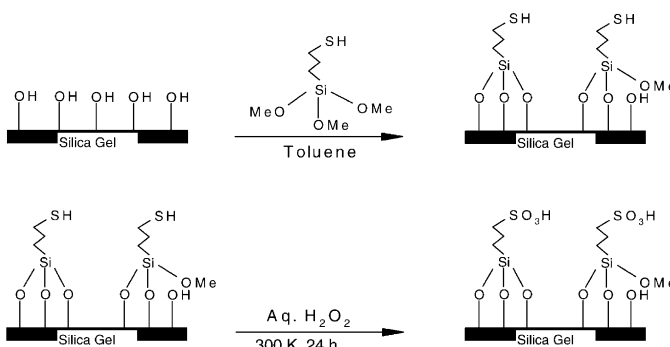


**S. Shylesh, Sahida Sharma, S.P. Mirajkar, A.P. Singh**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 219

Silica functionalised sulphonic acid groups: synthesis, characterization and catalytic activity in acetalization and acetylation reactions

Silica functionalised sulphonic acid groups were synthesized by the immobilization of propyl thiol groups and its subsequent oxidation to the corresponding acid using aq. H<sub>2</sub>O<sub>2</sub> as the oxidizing agent.

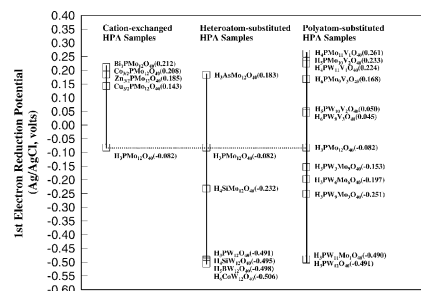


**In K. Song, Mark A. Barteau**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 229

Redox properties of Keggin-type heteropolyacid (HPA) catalysts: effect of counter-cation, heteroatom, and polyatom substitution

A map of first electron reduction potentials of Keggin-type heteropolyacids (HPAs) was established for HPA families with different counter-cation, polyatom, and heteroatom substitutions. The reduction potentials were determined by electrochemical method using Ag/AgCl as a reference electrode.

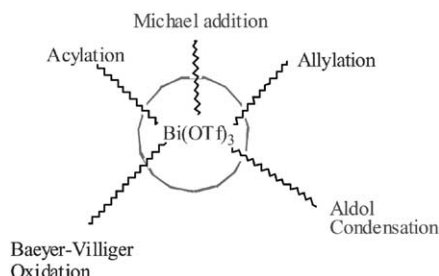


**B.M. Choudary, Ch. Sridhar, M. Sateesh, B. Sreedhar**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 237

Microencapsulated bismuth(III) triflate catalyst for organic transformations

A recoverable and reusable polymer encapsulated bismuth(III) triflate catalyst, designed and developed for the first time for effective allylation of aldehydes, Michael type addition of aliphatic amines to  $\alpha,\beta$ -ethylenic compounds, acylation of alcohols, Baeyer–Villiger oxidation and aldol condensation, exhibited truly heterogeneous nature throughout the reaction.

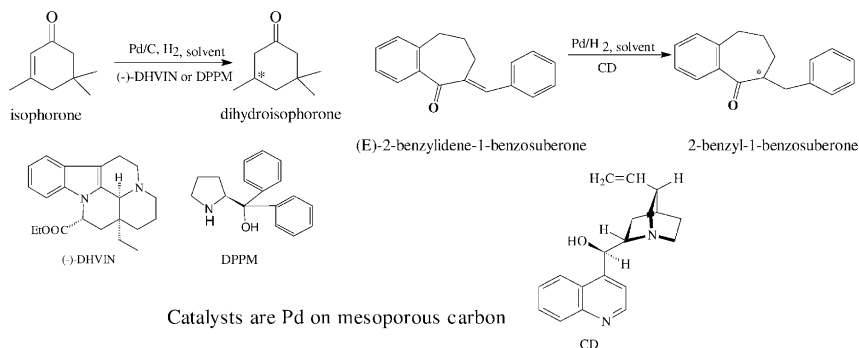




É. Sípos, G. Fogassy, A. Tungler, P.V. Samant, J.L. Figueiredo

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 245

Enantioselective hydrogenations with highly mesoporous carbon supported Pd catalysts

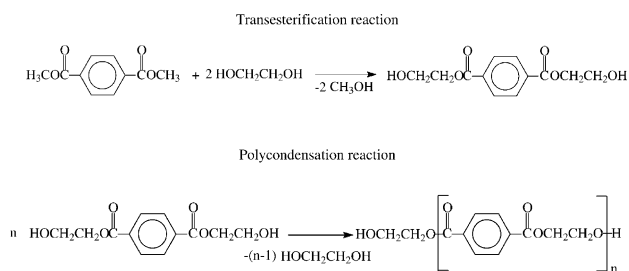


M. Di Serio, R. Tesser, A. Ferrara, E. Santacesaria

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 251

Heterogeneous basic catalysts for the transesterification and the polycondensation reactions in PET production from DMT

It was shown that both the calcined Al–Mg hydrotalcites and magnesium oxides are active in the dimethyl terephthalate (DMT) transesterification reaction with ethylene glycol (EG) and in the successive prepolymer polycondensation. The observed activities were compared to the results of characterisations of catalysts. Moreover, the obtained PETs have chemical and physical properties very close to those of commercial samples.

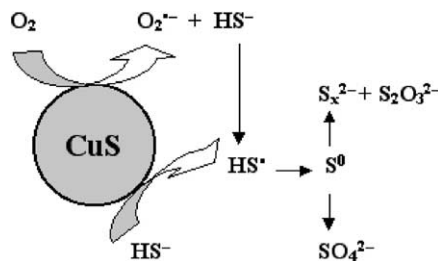


A.E. Raevskaya, A.L. Stroyuk, S.Ya. Kuchmii, A.I. Kryukov

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 259

Catalytic activity of CuS nanoparticles in hydrosulfide ions air oxidation

Spectral properties of colloidal CuS nanoparticles and their catalytic activity in hydrosulfide air oxidation have been investigated. It was found that the catalytic reaction occurs via chain-radical mechanism where CuS nanoparticles act as chain initiator.

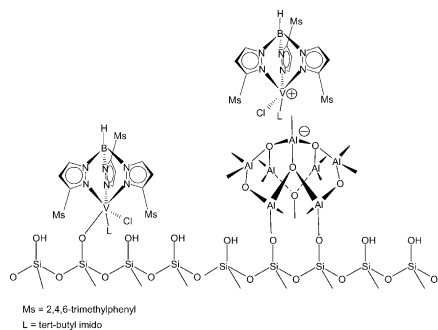


Adriana C.A. Casagrande, Tatiana T da R. Tavares, Maria Cristina A. Kuhn, Osvaldo L. Casagrande Jr., João H.Z. dos Santos, Toshiharu Teranishi

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 267

Tris(pyrazolyl)borate imido vanadium (V) compound immobilized on inorganic supports and its use in ethylene polymerization

Tris(pyrazolyl)borate imido vanadium (V) complex was immobilized on a series of inorganic support: SiO<sub>2</sub>, MAO-modified SiO<sub>2</sub>, SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>, MCM-41 and MgO and evaluated in ethylene polymerization. The highest activity was observed using silica as support. Resulting polymers were shown to be ultra-high molecular weight polyethylene.

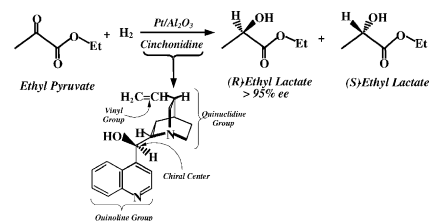


**Rene J. LeBlanc, Wei Chu,  
Christopher T. Williams**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 277

Surface Raman characterization of cinchonidine-modified platinum in ethanol: effects of liquid-phase concentration and co-adsorbed hydrogen

Surface-enhanced Raman spectroscopy has been utilized to probe the adsorption of the chiral modifier cinchonidine on platinum in ethanol at 25°C. The modifier is found to be strongly and irreversibly adsorbed through the quinoline portion of cinchonidine by  $\pi$ -bonding with the Pt surface. The degree of tilt of the quinoline group with respect to the surface increases as cinchonidine concentration increases. Addition of hydrogen appears to result in hydrogenation of the vinyl group on cinchonidine to form 10,11-dihydro-cinchonidine, resulting in a decrease in the tilt of the aromatic ring.

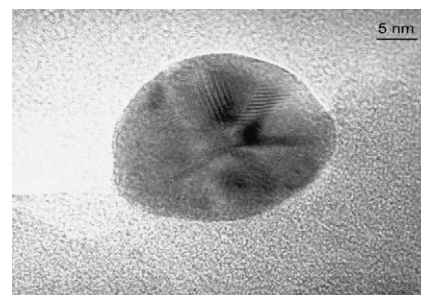


**Sheldon G. Shore, Errun Ding, Colin Park,  
Mark A. Keane**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 291

The application of  $\{(DMF)_{10}Yb_2[TM(CN)_4]_3\}_{\infty}$  (TM = Ni, Pd) supported on silica to promote gas phase phenol hydrogenation

Gas phase phenol hydrogenation activities/selectivities associated with Pd/SiO<sub>2</sub> prepared by Pd(NO<sub>3</sub>)<sub>2</sub> and Pd(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub> impregnation are compared with those delivered by Pd–Yb/SiO<sub>2</sub> prepared from a  $\{(DMF)_{10}Yb_2[Pd(CN)_4]_3\}_{\infty}$  precursor. Pd takes the form of nanoscale particles (see TEM image) while Yb is present as a thin film. The incorporation of Yb appreciably enhanced hydrogenation activity due to hydrogen transfer via surface Yb hydride.

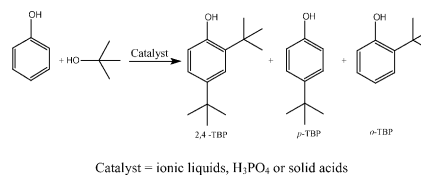


**Hao-Yu Shen, Zaher M.A. Judeh,  
Chi Bun Ching, Qing-Hua Xia**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 301

Comparative studies on alkylation of phenol with *tert*-butyl alcohol in the presence of liquid or solid acid catalysts in ionic liquids

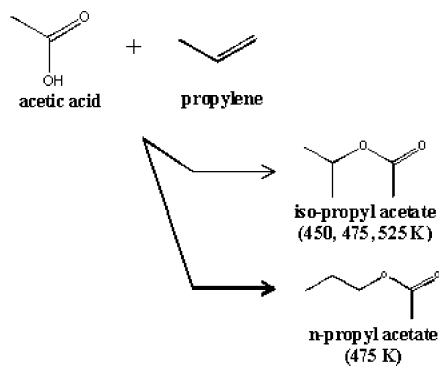
Alkylation of phenol with *tert*-butyl alcohol (TBA) was carried out in ionic liquids, H<sub>3</sub>PO<sub>4</sub> and some solid acidic catalysts, such as HZSM-5, H- $\beta$ , HPW and HPW/MCM-41. The use of ionic liquids was found to enhance the catalytic properties of the catalysts used.



**O. Kresnawahjuesa, R.J. Gorte, David White**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 309

The acylation of propene by acetic acid over H-[Fe]ZSM-5 and H-[Al]ZSM-5

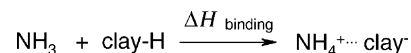


**M.P. Hart, D.R. Brown**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 315

Surface acidities and catalytic activities of acid-activated clays

The surface acidities of acid-activated clays K5 and K10 have been characterised by ammonia adsorption microcalorimetry. The success with which surface acidities measured in this way can be used to predict catalytic activities has been assessed using three model, acid-catalysed, test reactions.

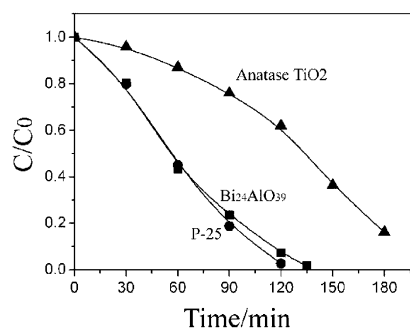


**W.F. Yao, X.H. Xu, J.T. Zhou, X.N. Yang, Y. Zhang, S.X. Shang, H. Wang, B.B. Huang**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 323

Photocatalytic property of sillenite  $\text{Bi}_{24}\text{AlO}_{39}$  crystals

$\text{Bi}_{24}\text{AlO}_{39}$  crystals with sillenite structures were prepared by the chemical solution decomposition (CSD) method. The photocatalytic activity of the prepared  $\text{Bi}_{24}\text{AlO}_{39}$  is high enough to photodegrade 20mg/l methyl orange in 2h, which is similar as that of P-25 and much better than that of anatase  $\text{TiO}_2$  prepared by us.

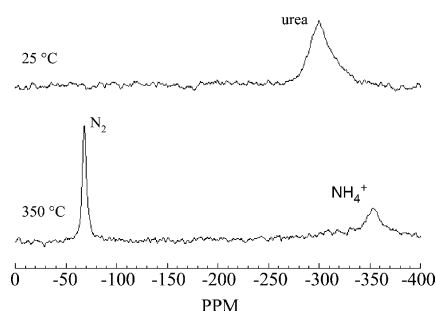


**Conrad A. Jones, Donald Stec, Sarah C. Larsen**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 329

Magnetic resonance studies of reactions of urea and nitric oxide on FeZSM-5, HZSM-5 and silicalite

Solid state NMR experiments were used to investigate the reactions of urea and NO on H- and FeZSM-5 demonstrating the potential of these materials for the selective catalytic reduction of NO with urea.

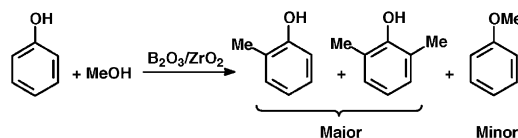


**Kusum M. Malshe, Pratap T. Patil, Shubhangi B. Umbarkar, Mohan K. Dongare**

*Journal of Molecular Catalysis A: Chemical* 212 (2004) 337

Selective C-methylation of phenol with methanol over borate zirconia solid catalyst

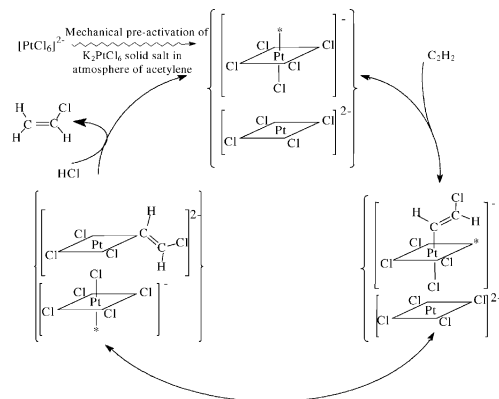
Preferential C-alkylated products i.e. *o*-cresol and 2,6-xyleneol were obtained in high yields in methylation of phenol using borate zirconia solid acid catalyst prepared by wet impregnation method. The higher activity/selectivity and stability of the catalysts is correlated with composition and structure. The mechanism of selective *ortho*-alkylation was investigated using FTIR studies.



Serge A. Mitchenko, Eugene V. Khomutov,  
Alexander A. Shubin, Yuri M. Shul'ga

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 345

Catalytic hydrochlorination of acetylene by gaseous HCl on the surface of mechanically pre-activated  $K_2PtCl_6$  salt

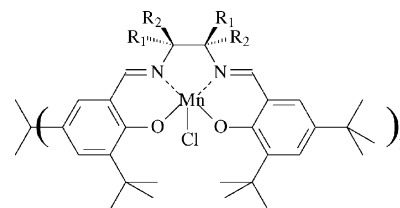


Liu Xinwen, Tang Ning, Liu Weisheng,  
Tan Minyu

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 353

Synthesis, catalytic activity and recycle of novel dimeric salen-Mn(III) complexes in asymmetric epoxidation

Novel chiral dimeric salen-Mn(III) complexes were synthesized and then investigated in the catalytic epoxidation of unfunctionalized alkenes. High activity and enantioselectivity were achieved. The dimer formation enhanced the catalyst's reactivity and stability without compromising its enantioselectivity. Catalyst **3a** could be easily recovered and reused for several cycles under the mild reaction conditions.



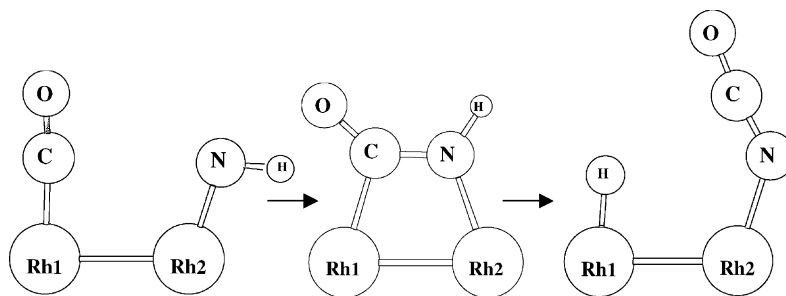
**3a:**  $R_1 = H$ ,  $R_2 = Ph$ ; **3b:**  $R_1 - R_1 = -(CH_2)_4-$ ,  $R_2 = H$ .

Ricardo M. Ferullo, Norberto J. Castellani

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 359

NCO formation from CO and NH species over  $Rh_2$ . A density functional theory study

The DFT formalism was used to study the reaction between coadsorbed CO and NH species to form NCO over  $Rh_2$ . A precursor state towards the NCO formation was found.



Cuiping Yu, Lifang Zhang, Zhiquan Shen

*Journal of Molecular Catalysis A: Chemical* 212  
(2004) 365

Ring-opening polymerization of 2,2-dimethyltrimethylene carbonate using rare earth tris(4-tert-butylphenolate)s as a single component initiator

Single component rare earth tris(4-tert-butylphenolate)s ( $Ln(OTBP)_3$ ) as initiators for the ring-opening polymerization of 2,2-dimethyltrimethylene carbonate are reported for the first time. Lanthanum tris(4-tert-butylphenolate)s has higher activity and gives higher molecular weight polycarbonate under quite mild conditions.

