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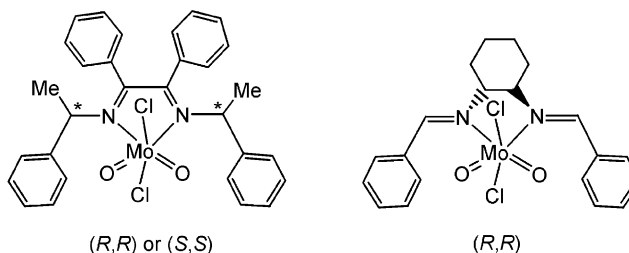
Articles

Sandra Gago, José E. Rodríguez-Borges, Cátia Teixeira, Ana M. Santos, Jin Zhao, Martyn Pillinger, Carla D. Nunes, Željko Petrovski, Teresa M. Santos, Fritz E. Kühn, Carlos C. Romão, Isabel S. Gonçalves

Journal of Molecular Catalysis A: Chemical 236 (2005) 1

Synthesis, characterization and catalytic studies of bis(chloro)dioxomolybdenum(VI)-chiral diimine complexes

Six-coordinate dioxomolybdenum(VI) complexes of the type $[\text{MoO}_2\text{Cl}_2\text{L}]$ containing bidentate chiral ligands were evaluated as catalysts for the asymmetric epoxidation of *cis*- and *trans*- β -methylstyrene by *tert*-butylhydroperoxide at either room temperature or 55°C. The reactions proceeded with high retention of olefin configuration and high selectivity to the epoxide, but only for *cis*- β -methylstyrene were significant enantiomeric excesses obtained.

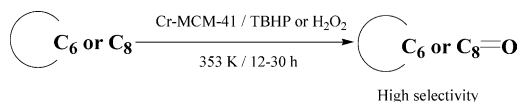


S. Samanta, N.K. Mal, A. Bhaumik

Journal of Molecular Catalysis A: Chemical 236 (2005) 7

Mesoporous Cr-MCM-41: An efficient catalyst for selective oxidation of cycloalkanes

Mesoporous Cr-MCM-41 (with different Si:Cr mole ratios) have been synthesized by using the self-assembly of cationic surfactant as structure directing agent. This material showed excellent activity in one-pot liquid phase selective oxidation of cyclohexane and cyclooctane to cyclohexanone and cyclooctanone, respectively, using dilute aqueous peroxide oxidants.

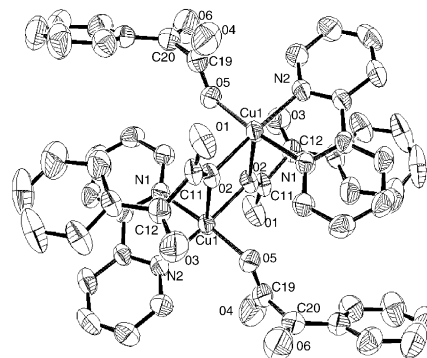


József Kaizer, Róbert Csonka, Gábor Speier, Michel Giorgi, Marius Réglér

Journal of Molecular Catalysis A: Chemical 236 (2005) 12

Synthesis, structure and catalase-like activity of new dicopper(II) complexes with phenylglyoxylate and benzoate ligands

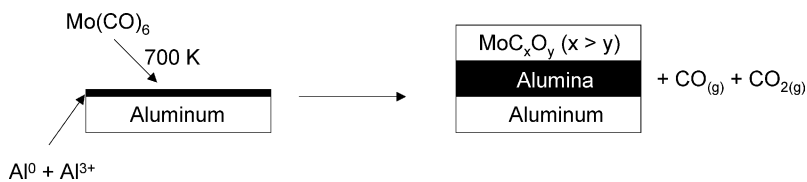
Dimeric $\text{Cu}_2(\text{bpy})_2(\text{phga})_4$ and $\text{Cu}_2(\text{ba})_4(\text{bpy})_2$ complexes were isolated and characterized. Single crystal X-ray structure of the $\text{Cu}_2(\text{bpy})_2(\text{phga})_4$ complex is also reported. These complexes were found to present catalase-like activity.



Y. Wang, F. Gao, W.T. Tysoe

Journal of Molecular Catalysis A: Chemical 236 (2005) 18

Interaction of molybdenum hexacarbonyl with metallic aluminum at high temperatures: Carbide and alloy formation

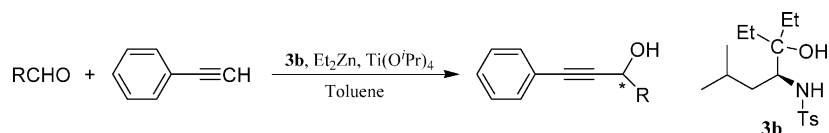


Zhi-jian Han, Chao-shan Da, Zhao-qing Xu, Ming Ni, Rui Wang

Journal of Molecular Catalysis A: Chemical 236 (2005) 32

The asymmetric addition of phenylacetylene to aldehydes catalyzed by L-leucine derived chiral sulfonamide alcohol ligands

The asymmetric addition of phenylacetylene to aldehydes catalyzed by L-leucine derived chiral sulfonamide alcohol ligands.

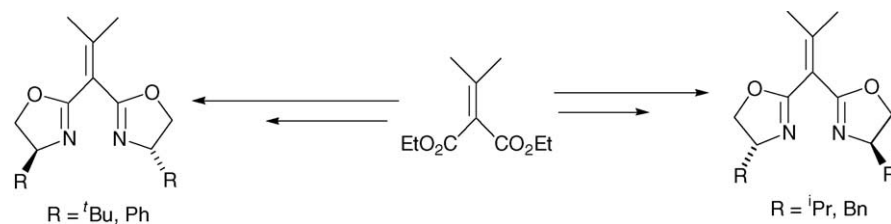


Elisabete da Plama Carreiro, Serghei Chercheja, Anthony J. Burke, J.P. Prates Ramalho, Ana Isabel Rodrigues

Journal of Molecular Catalysis A: Chemical 236 (2005) 38

Isbut-Box: A new chiral C_2 symmetric bis-oxazoline for catalytic enantioselective synthesis

The synthesis of a new class of chiral non-racemic bisoxazoline ligand and their evaluation in the catalytic asymmetric Cu(I) catalysed cyclopropanation reaction is reported in this paper.

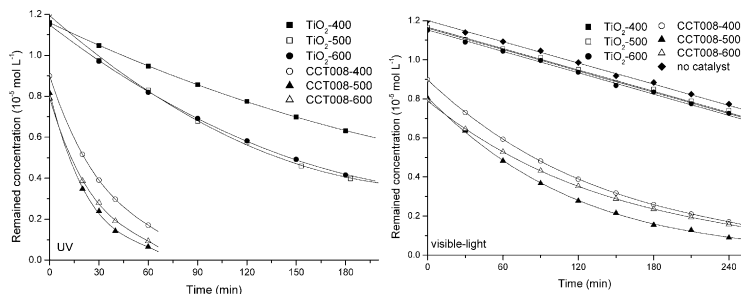


L. Lin, W. Lin, Y.X. Zhu, B.Y. Zhao, Y.C. Xie, Y. He, Y.F. Zhu

Journal of Molecular Catalysis A: Chemical 236 (2005) 46

Uniform carbon-covered titania and its photocatalytic property

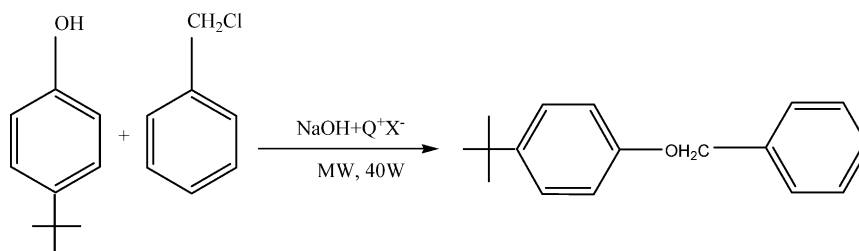
Carbon-covered titania (CCT) was prepared *via* pyrolysis of sucrose highly dispersed on the surface of titania. The as-prepared CCT shows much higher catalytic activity for MB's photodegradation than pure titania under UV illumination. In addition, MB can be decomposed over CCT under visible light illumination, whereas it is simply bleached over pure titania at the same condition.



Ganapati D. Yadav, Priyal M. Bisht

Journal of Molecular Catalysis A: Chemical 236 (2005) 54

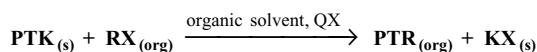
Fundamental analysis of microwave irradiated liquid–liquid phase transfer catalysis (MILL-PTC): Simultaneous measurement of rate and exchange equilibrium constants in selective *O*-alkylation of *p*-*tert*-butylphenol with benzyl chloride

**Maw-Ling Wang, Wei-Hung Chen, Feng-Sheng Wang**

Journal of Molecular Catalysis A: Chemical 236 (2005) 65

Kinetic study of synthesizing *N*-butylphthalimide under solid–liquid phase-transfer catalysis conditions

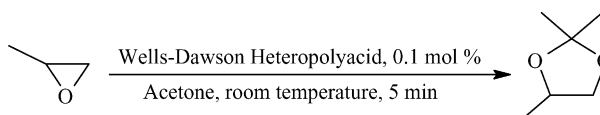
The technique of solid–liquid phase transfer catalysis (SL-PTC) was applied to synthesize *N*-butylphthalimide (PTR) from the reaction of 1-bromobutane and potassium salt of phthalimide (PTK) to obtain high yield and avoid hydration.

**Guixian Li, Bo Wang, Jianming Wang, Yong Ding, Liang Yan, Jishuan Suo**

Journal of Molecular Catalysis A: Chemical 236 (2005) 72

Efficient and highly-selective cycloaddition of epoxides with carbonyl compound over Wells–Dawson type heteropolyacids

Wells–Dawson Heteropoly acids ($\text{H}_{6+n}\text{P}_2\text{Mo}_{18-n}\text{V}_n\text{O}_{62}$) ($n = 0-2, 4$) have proved to be efficient heterogeneous catalysts for the reaction of epoxides with carbonyl compounds to form 1,3-dioxolane derivatives.

**Deepak B Akolekar, Suresh K Bhargava**

Journal of Molecular Catalysis A: Chemical 236 (2005) 77

Investigations on gold nanoparticles in mesoporous and microporous materials

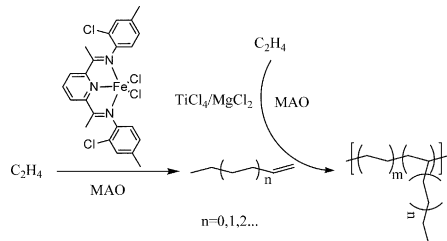
The gold nanoparticles in different high surface area mesoporous and microporous materials were prepared using sol–gel and hydrothermal crystallization methods. For investigating the characteristics behaviour of nano gold particles in the mesoporous and microporous materials, Au–Al–MCM-41, Au–ZSM-5 and Au–LSX were prepared with different framework composition and concentrations of gold nanoparticles. The Au–Al–MCM-41, Au–ZSM-5 and Au–LSX samples were characterized using the BET, FTIR, ICP-MS, XAS, XPS, TEM and XRD. The XPS measurements indicate that the presence of gold species in different oxidation state and concentration of gold metal species varies over the surfaces of as-synthesized and calcined gold containing mesoporous and microporous materials.

Zhicheng Zhang, Zhanxia Lu, Shangtao Chen, Huayi Li, Xiaofan Zhang, Yingying Lu, Youliang Hu

Journal of Molecular Catalysis A: Chemical 236 (2005) 87

Synthesis of branched polyethylene from ethylene stock by an interference-free tandem catalysis of $\text{TiCl}_4/\text{MgCl}_2$ and iron catalyst

An interference-free tandem catalysis, based on $[(2\text{-ArN}=\text{C}(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N})\text{FeCl}_2$ ($\text{Ar} = 2\text{-Cl-4-CH}_3\text{C}_6\text{H}_3$)/MAO and $\text{TiCl}_4/\text{MgCl}_2/\text{MAO}$, was used for the synthesis of branched polyethylene with ethylene as the only monomer stock. The deactivation due to the side reactions of catalysts and cocatalysts could be totally avoided because MAO was used as the sole cocatalyst. By changing the reaction conditions and Fe/Ti molar ratio, a series of branched polyethylene with different branching degrees were effectively produced.

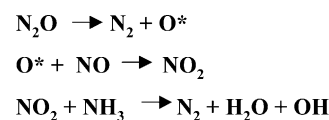


Seong Moon Jung, Olivier Demoulin, Paul Grange

Journal of Molecular Catalysis A: Chemical 236 (2005) 94

The study of a synergetic effect over a H-ZSM-5/ V_2O_5 hybrid catalyst on SCR reaction

The synergetic effect over a H-ZSM-5/ V_2O_5 hybrid catalyst on SCR reaction can be explained by that V_2O_5 plays a role as a supplier of oxygen source through N_2O formation, while H-ZSM-5 decomposes N_2O into N_2 and α -oxygen contributing to the increase of the apparent SCR activity.

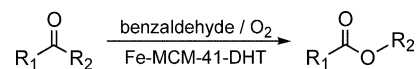


Tomonori Kawabata, Yoshihiko Ohishi, Satoko Itsuki, Naoko Fujisaki, Tetsuya Shishido, Ken Takaki, Qinghong Zhang, Ye Wang, Katsuomi Takehira

Journal of Molecular Catalysis A: Chemical 236 (2005) 99

Iron-containing MCM-41 catalysts for Baeyer–Villiger oxidation of ketones using molecular oxygen and benzaldehyde

Fe-MCM-41-DHT exhibited a high catalytic activity for Baeyer–Villiger (B–V) oxidation of ketones using molecular oxygen and benzaldehyde. The prominent performance of the Fe-MCM-41-DHT could be ascribed to both tetrahedrally coordinated Fe^{3+} incorporated inside the framework of MCM-41 and its uniform nano-order mesopores allowing the access of bulky compounds to the active sites.

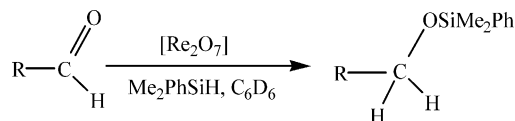


Beatriz Royo, Carlos C. Romão

Journal of Molecular Catalysis A: Chemical 236 (2005) 107

Reduction of carbonyl groups by high-valent rhenium oxides

The catalytic activity of high valent oxo-rhenium derivatives for hydrosilylation of aldehydes and ketones has been investigated. We have found that methyltrioxorhenium(VII) and oxotrichlorobis(triphenylphosphine)rhenium(V) are effective catalysts for the hydrosilylation of aldehydes and ketones with dimethylphenylsilane.

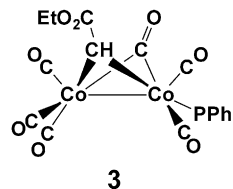
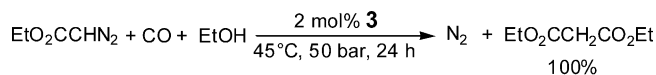


Robert Tuba, Eszter Fördös, Ferenc Ungváry

Journal of Molecular Catalysis A: Chemical 236 (2005) 113

Preparation of triphenylphosphane substituted ethoxycarbonylcarbene-bridged dicobalt carbonyl complexes and their application as catalyst precursors in the carbonylation of ethyl diazoacetate in the carbonylation of ethyl diazoacetate to diethyl malonate

Triphenylphosphane substituted derivatives $\text{Co}_2(\text{CO})_6(\text{CHCO}_2\text{Et})(\text{PPh}_3)$ (**3**) and $\text{Co}_2(\text{CO})_5(\text{CHCO}_2\text{Et})(\text{PPh}_3)_2$ (**4**) were prepared from the known $\text{Co}_2(\text{CO})_7(\text{CHCO}_2\text{Et})$ and $\text{Co}_2(\text{CO})_6(\text{CHCO}_2\text{Et})_2$ complexes and were tested along with other phosphane-substituted cobalt carbonyl complexes as catalyst precursors in the carbonylation reaction of ethyl diazoacetate into diethyl malonate in the presence of ethanol.

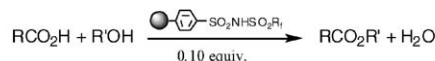
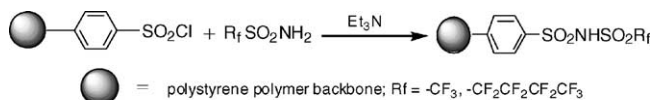


Jiezhao Xiao, Zhengbo Zhang, Jin Nie

Journal of Molecular Catalysis A: Chemical 236 (2005) 119

Preparation, characterization and catalytic activity of polystyrene with pendent perfluoroalkylsulfonamide groups

A new type of fluorinated strongly acidic polymers has been prepared and characterized. The catalytic activity and recycling ability have been examined for direct esterification of carboxylic acids with alcohols. It is indicated that the PPFSA was a strongly acidic polymer, which could be tolerant of high temperature, and an effective catalyst for direct condensation of carboxylic acids and alcohols.

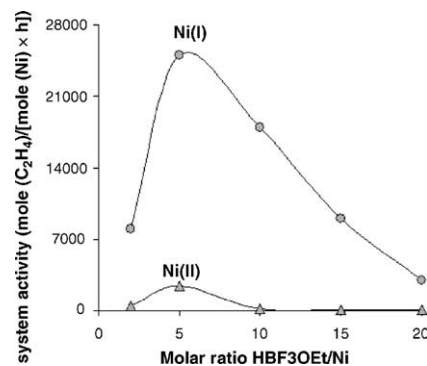


V.V. Saraev, P.B. Kraikivskii, S.N. Zelinskiy, D.A. Matveev, A.I. Vilms, A.V. Rohin, K. Lammertsma

Journal of Molecular Catalysis A: Chemical 236 (2005) 125

Influence of alcohols on the formation of the nickel complexes active in ethene oligomerization in the catalytic system $\text{Ni}(\text{PPh}_3)_4/\text{BF}_3 \cdot \text{OEt}_2$

Coordinationally unsaturated Ni(I) complexes were shown to be the active catalysts for ethylene oligomerization, whereas the Ni(II) hydrides were shown to be inactive.

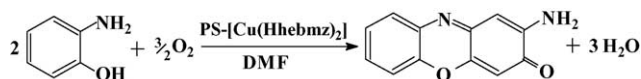


Mannar R. Maurya, Sweta Sikarwar, Trissa Joseph, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 236 (2005) 132

Bis(2-[α -hydroxyethyl]benzimidazolato)copper(II) anchored onto chloromethylated polystyrene for the biomimetic oxidative coupling of 2-aminophenol to 2-aminophenoxazine-3-one

Oxidative coupling of 2-aminophenol (OAP) to 2-aminophenoxazine-3-one (APX) catalyzed by polymer-anchored bis(2-[α -hydroxyethyl]benzimidazolato)copper(II) (PS-[Cu(hebzm)₂]) in presence of air at 70°C in DMF has been reported.

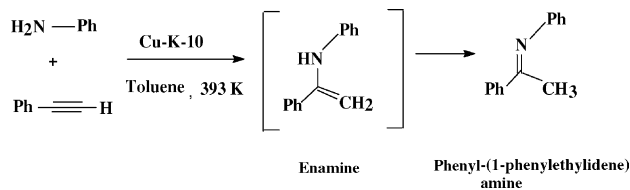


Trissa Joseph, G.V. Shanbhag, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 236 (2005) 139

Copper(II) ion-exchanged montmorillonite as catalyst for the direct addition of N-H bond to CC triple bond

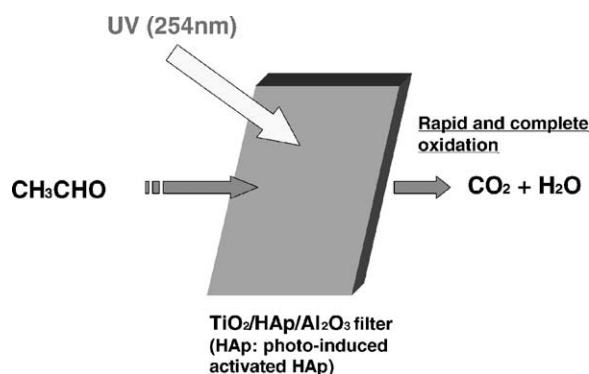
An efficient synthesis of phenyl-(1-phenylethylidene)amine using copper(II) ion-exchanged montmorillonite clay is demonstrated. The reaction is highly regio-selective and proceeded smoothly to completion.



Harumitsu Nishikawa, Shinji Kato, Takahiro Ando

Journal of Molecular Catalysis A: Chemical 236 (2005) 145

Rapid and complete oxidation of acetaldehyde on TiO₂ photocatalytic filter supported by photo-induced activated hydroxyapatite

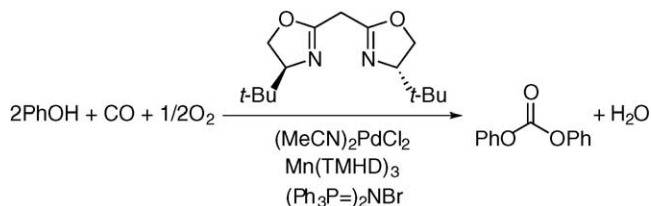


Hiroyuki Yasuda, Keiji Watarai, Jun-Chul Choi, Toshiyasu Sakakura

Journal of Molecular Catalysis A: Chemical 236 (2005) 149

Effects of bulky ligands and water in Pd-catalyzed oxidative carbonylation of phenol

The use of 2,2'-bioxazolyl ligands with bulky substituents at the 4,4'-position effectively accelerated the Pd-catalyzed oxidative carbonylation of phenol to produce diphenyl carbonate (DPC); the TONs of DPC were methyl < benzyl < *iso*-butyl < *tert*-butyl. The addition of molecular sieve 3A prevented CO₂ formation, partly due to suppression of the reaction between CO and water.

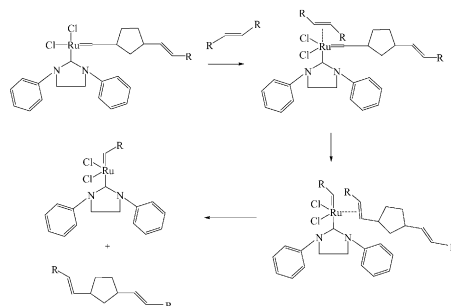


Serguei Fomine, Joel Vargas Ortega, Mikhail A. Tlenkopatchev

Journal of Molecular Catalysis A: Chemical 236 (2005) 156

Computational modeling of ruthenium alkylidene mediated olefin metathesis. A DFT study of reaction pathways for the ring-opening cross-metathesis of norbornene with olefins

The chain transfer reaction pathways from ring-opened norbornene to ethylene and 1,4-dichloro-2-butene (DB) using (1,3-diphenyl-4,5-dihydroimidazol-2-ylidene) (PCy₃)Cl₂Ru=CHPh catalyst (**I**) have been studied at B3LYP/LACVP** level of theory. The calculations show that compared to ethylene, DB binds less strongly to the 14 electron Ru-alkylidene catalyst to form the metallacycle. The activation energies found for both chain transfer reactions, if any, are very low making the kinetic factor to be of little importance.



Biju M. Devassy, F. Lefebvre, Walter Böhringer, Jack Fletcher, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 236 (2005) 162

Synthesis of linear alkyl benzenes over zirconia-supported 12-molybdophosphoric acid catalysts

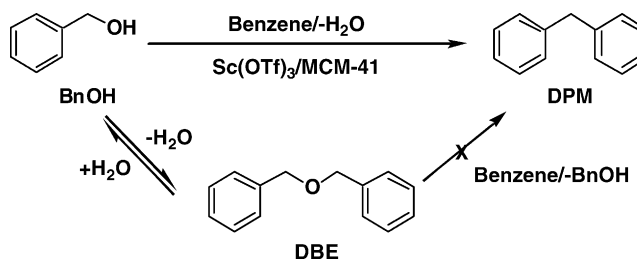
The paper deals with the preparation and characterization of zirconia supported 12-molybdophosphoric acid catalysts and its application in liquid-phase linear alkyl benzene synthesis by the reaction of benzene with 1-octene and 1-dodecene. The most active catalyst, 15% MPA/ZrO₂ calcined at 700°C gave >90% olefin conversions with selectivity to 2-phenyl octane, 55% and 2-phenyl dodecane, 45%.

Kshudiram Mantri, Kenichi Komura, Yoshihiro Kubota, Yoshihiro Sugi

Journal of Molecular Catalysis A: Chemical 236 (2005) 168

Friedel–Crafts alkylation of aromatics with benzyl alcohols catalyzed by rare earth metal triflates supported on MCM-41 mesoporous silica

Liquid phase benzylation of aromatics, such as benzene, toluene, *p*-xylene, mesitylene and naphthalene, with benzyl alcohols was examined using rare earth metal triflates, Sc(OTf)₃, Hf(OTf)₄, La(OTf)₃, and Yb(OTf)₄, supported on MCM-41 mesoporous silica. Sc(OTf)₃/MCM-41 had the highest catalytic performance among the triflates. The benzylation of benzene proceeds principally to give diphenylmethane (DPM) through direct benzylation with benzyl alcohol (BnOH). Dibenzyloxy ether (DBE) is formed as a by-product, and it participates in the benzylation with the decrease in BnOH after the hydrolysis.

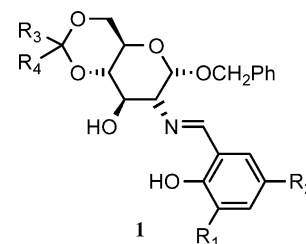


Maria Elena Cucciolito, Raffaella Del Litto, Giuseppina Roviello, Francesco Ruffo

Journal of Molecular Catalysis A: Chemical 236 (2005) 176

O,N,O'-tridentate ligands derived from carbohydrates in the V(IV)-promoted asymmetric oxidation of thioanisole

O,N,O'-tridentate ligands (**1**) derived from sugars have been obtained by condensing 2-amino- α -D-pyranosides with several 3,5-disubstituted-2-hydroxybenzaldehydes. The efficiency of the imines in the V(IV)-promoted asymmetric oxidation of thioanisole has been examined and yields up to 60% have been achieved.



Junjiang Zhu, Dehai Xiao, Jing Li, Xiangguang Yang, Yue Wu

Journal of Molecular Catalysis A: Chemical 236 (2005) 182

Kinetics and mechanism of NO decomposition over La_{0.4}Sr_{0.6}Mn_{0.8}Ni_{0.2}O₃ perovskite-type oxides

The kinetic equation of NO decomposition over perovskite-type oxide is deduced. The reaction order for NO is 1 in the range 0.5–2.0 vol.% NO/He, while it varies from –0.24 to –0.08 for O₂ (0–6 vol.% O₂/He), depending on the temperature. The item $K_{-6}(K_{-7})^{1/2}P_{\text{NO}}(P_{\text{O}_2})^{1/2}$, which reflects the reciprocity of O₂ and NO in the reaction, is introduced in the kinetics for the first time.

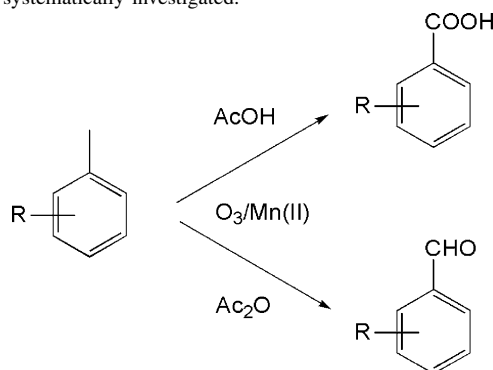
$$r = \frac{k_3 K_1 K_2 P_{\text{NO}}^2 [L]}{1 + K_1 P_{\text{NO}} + (K_{-5} K_{-6} K_{-7}^{1/2} / K_1) P_{\text{O}_2}^{1/2} + K_{-6} K_{-7}^{1/2} P_{\text{NO}} P_{\text{O}_2}^{1/2}}$$

**Mario Waser, Walther G. Jary,
Peter Pöchlauer, Heinz Falk**

Journal of Molecular Catalysis A: Chemical 236
(2005) 187

Concerning chemistry, reactivity, and mechanism of transition metal catalysed oxidation of benzylic compounds by means of ozone

Chemistry, reactivity, and mechanism of transition metal catalysed oxidation of benzylic compounds by means of ozone were systematically investigated.

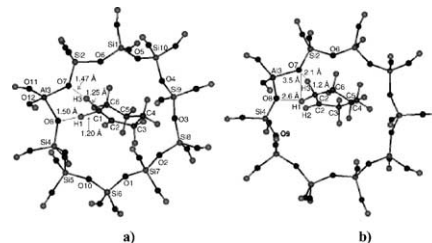


Angeles Cuán, José Manuel Martínez-Magadán, Isidoro García-Cruz, Marcelo Galván

Journal of Molecular Catalysis A: Chemical 236
(2005) 194

DFT—Quantum chemical study of the HZSM-5-cyclohexene interaction pathways

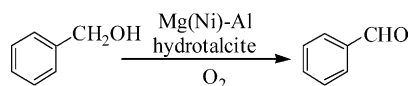
A theoretical analysis of the interaction between cyclohexene and HZSM-5 zeolite model systems is presented. Two different reaction pathways are fully characterized: hydrogen exchange and proton addition to the double bond of the olefin. The comparisons of two representations of the catalytic site indicate that a ring model gives rise to a more ionic intermediate species. These intermediates are characterized as minima in the PES, but they are destabilized with respect to the corresponding physisorbed complexes. In addition, the structures of the transition states for both trajectories are determined. Transition states geometries involved in, (a) the hydrogen exchange reaction and (b) proton addition to the cyclohexene double bond.



**Tomonori Kawabata, Yuriko Shinozuka,
Yoshihiko Ohishi, Tetsuya Shishido,
Ken Takaki, Katsuomi Takehira**

Journal of Molecular Catalysis A: Chemical 236
(2005) 206

Nickel containing Mg-Al hydrotalcite-type anionic clay catalyst for the oxidation of alcohols with molecular oxygen

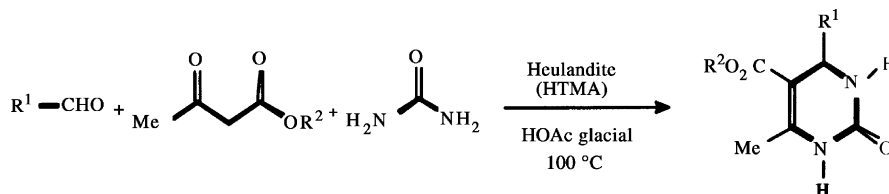


**Mahmood Tajbakhsh, Bagher Mohajerani,
Majid M. Heravi, Amir N. Ahmadi**

Journal of Molecular Catalysis A: Chemical 236
(2005) 216

Natural HEU type zeolite catalyzed Biginelli reaction for the synthesis of 3,4-dihydropyrimidin-2(1H) one derivatives

A new method for Biginelli reaction via a heterogenous catalyst has been developed. This method uses natural Heulandite type zeolite (HTMA) as a catalyst for the one pot condensation of an aldehyde, urea and a 1,3-dicarbonyl compound under mild conditions in excellent yields.

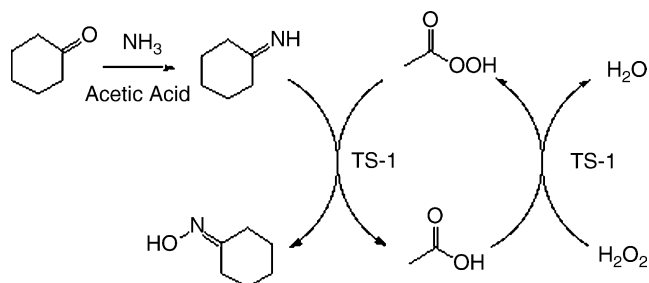


Tawan Sooknoi, Veerachai Chitrannuwatkul

Journal of Molecular Catalysis A: Chemical 236 (2005) 220

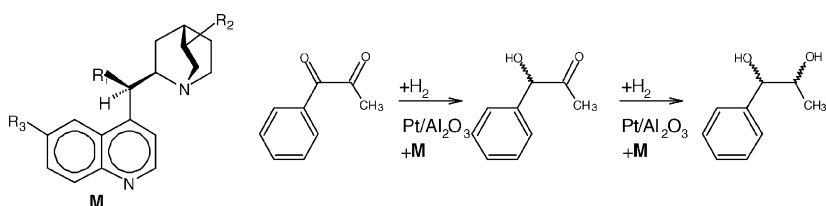
Ammoximation of cyclohexanone in acetic acid using titanium silicalite-1 catalyst: Activity and reaction pathway

In the reaction using acetic as a solvent, peracetic acid is formed and served as an oxidising agent. Also, the reaction of cyclohexanone with ammonia is enhanced and thus cyclohexanone oxime is formed by the oxidation of its corresponding imine.

**Igor Busygin, Esa Toukonniitty, Reko Leino, Dmitry Yu. Murzin**

Journal of Molecular Catalysis A: Chemical 236 (2005) 227

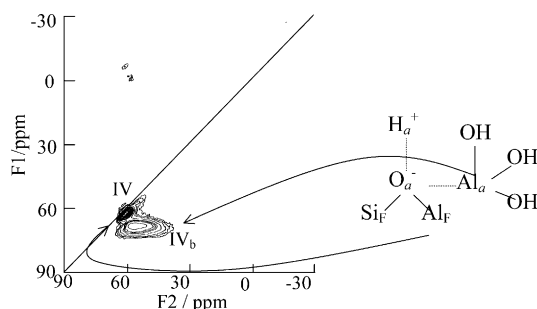
Effect of modifier structure in asymmetric 1-phenylpropane-1,2-dione hydrogenation

**Naonobu Katada, Shinichi Nakata, Sumio Kato, Koji Kanehashi, Koji Saito, Miki Niwa**

Journal of Molecular Catalysis A: Chemical 236 (2005) 239

Detection of active sites for paraffin cracking on USY zeolite by ^{27}Al MQMAS NMR operated at high magnetic field 16 T

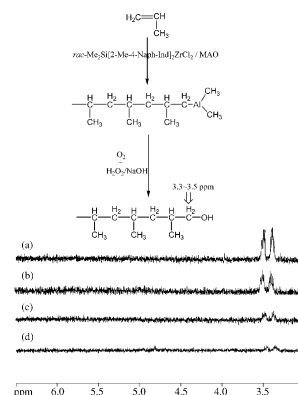
^{27}Al MAS and 3QMAS NMR at a high magnetic field (16 T) detected a tetra-coordinated species of extra-framework Al with a large structural anisotropy (IV_b), which was a candidate of active species for paraffin cracking on USY zeolite.

**Guoqiang Fan, Jin-Yong Dong**

Journal of Molecular Catalysis A: Chemical 236 (2005) 246

An examination of aluminum chain transfer reaction in *rac*-Me₂Si[2-Me-4-Naph-Ind]₂ZrCl₂/MAO-catalyzed propylene polymerization and synthesis of aluminum-terminated isotactic polypropylene with controlled molecular weight

Chain transfer to the aluminum cocatalyst was found to be the predominant chain transfer reaction in propylene polymerization mediated by *rac*-dimethylsilanediybis(2-methyl-4-naphthyl) indenyl-zirconium dichloride (*rac*-Me₂Si[2-Me-4-Naph-Ind]₂ZrCl₂)/methylaluminoxane (MAO) catalyst system. By finely tuning the polymerization conditions, this predominant aluminum transfer reaction was directed to prepare aluminum-terminated isotactic polypropylene (*i*-PP) with high end-group selectivity and controlled and narrowly distributed molecular weight. ^1H NMR spectra of polypropylenes prepared at 10°C with Al/Zr ratio of (a) 10000, (b) 5000, (c) 1500 and (d) 500.



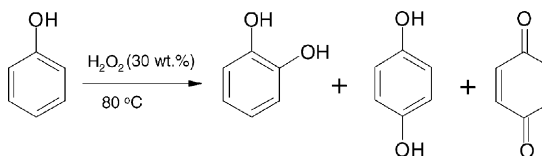
^1H NMR spectra of polypropylenes prepared at 10°C with Al/Zr ratio of (a) 10000, (b) 5000, (c) 1500 and (d) 500.

**S. Shylesh, T. Radhika, K. Sreeja Rani,
S. Sugunan**

Journal of Molecular Catalysis A: Chemical 236
(2005) 253

Synthesis, characterization and catalytic activity
of Nd_2O_3 supported V_2O_5 catalysts

Rare-earth neodymia supported Nd-V-O catalysts synthesized by wet impregnation method reveals the presence of two kinds of vanadia species on the support surfaces—one as highly dispersed species at lower loadings (<9%) and the other as an orthovanadate species at higher loadings, where the former exhibits promising catalytic behaviour in the liquid phase hydroxylation reaction of phenol.



Monirul Islam, Bidyut Saha, Asim K. Das

Journal of Molecular Catalysis A: Chemical 236
(2005) 260

Kinetics and mechanism of 2,2'-bipyridyl and
1,10-phenanthroline-catalysed chromium(VI)
oxidation of D-fructose in aqueous micellar media

