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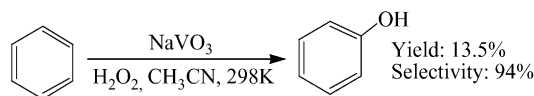
Articles

**Min Jian, Liangfang Zhu, Jinyue Wang,
Jin Zhang, Guiying Li, Changwei Hu**

*Journal of Molecular Catalysis A: Chemical 253
(2006) 1*

Sodium metavanadate catalyzed direct hydroxylation of benzene to phenol with hydrogen peroxide in acetonitrile medium

Sodium metavanadate catalyzed direct hydroxylation of benzene to phenol with hydrogen peroxide in acetonitrile medium was studied. A satisfactory yield of 13.5% with a selectivity of 94% was obtained. A free radical mechanism involving the state variation of vanadium species was proposed based on in situ ^{51}V -NMR.



Biju M. Devassy, S.B. Halligudi

*Journal of Molecular Catalysis A: Chemical 253
(2006) 8*

Effect of calcination temperature on the catalytic activity of zirconia-supported heteropoly acids

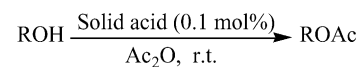
Zirconia-supported silicotungstic acid (15%) calcined at 750 °C shown to be more active catalyst compared to phosphotungstic acid-based catalyst for acylation and alkylation of aromatic compounds and catalytic activity decreases with an increase in support calcination temperature.

**Majid M. Heravi, Farahnaz K. Behbahani,
Fateme F. Bamoharram**

*Journal of Molecular Catalysis A: Chemical 253
(2006) 16*

$\text{H}_{14}[\text{NaP}_5\text{W}_{30}\text{O}_{110}]$: A heteropoly acid catalyzed acetylation of alcohols and phenols in acetic anhydride

A trace amount of $\text{H}_{14}[\text{NaP}_5\text{W}_{30}\text{O}_{110}]$ (0.1 mol%) has been effectively used as heteropoly acid catalyst for acetylation of alcohols and phenols with acetic anhydride at room temperature.

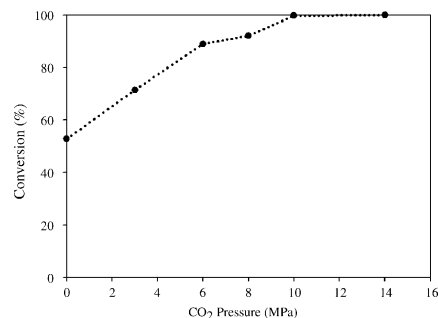


Joongjai Panpranot, Kunnika Phandinthong, Piyasan Prasertdam, Masashi Hasegawa, Shin-ichiro Fujita, Masahiko Arai

Journal of Molecular Catalysis A: Chemical 253 (2006) 20

A comparative study of liquid-phase hydrogenation on Pd/SiO₂ in organic solvents and under pressurized carbon dioxide: Activity change and metal leaching/sintering

Compared to the use of organic solvents or solvent less, the use of high-pressure CO₂ enhanced the hydrogenation activity of Pd/SiO₂ catalyst. However, metal sintering and leaching in the presence of high-pressure CO₂ were comparable to those in organic solvents.

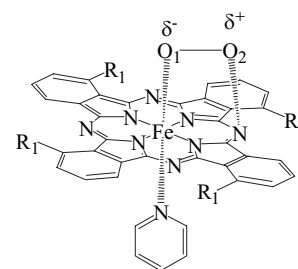


Liang Yang, Mei-Jin Lin, Xiao-Li Zhu, Xiu-Zhi Xu, Jun-Dong Wang

Journal of Molecular Catalysis A: Chemical 253 (2006) 25

Spectra and stabilities of α -substituted phthalocyaninatoirons

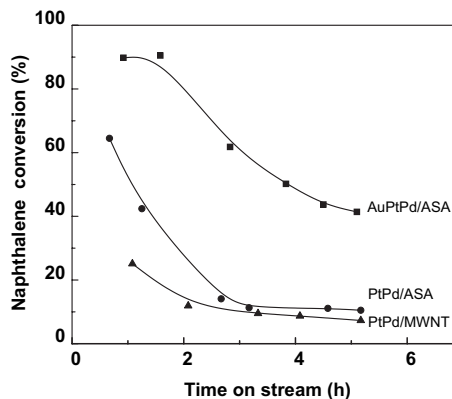
Three aryloxy (alkoxy) α -substituted phthalocyaninatoirons (FePcs) were prepared and their UV-vis spectra in air or by adding of peroxide showed a new band at the red side of the Q band which can be assigned to a complexes of phthalocyaninatoirons with oxygen or peroxide. The appearance of this band related to the instability of these FePcs so their decomposition was also studied, by the benzoylperoxide oxidation.



B. Pawelec, V. La Parola, S. Thomas, J.L.G. Fierro

Journal of Molecular Catalysis A: Chemical 253 (2006) 30

Enhancement of naphthalene hydrogenation over PtPd/SiO₂-Al₂O₃ catalyst modified by gold

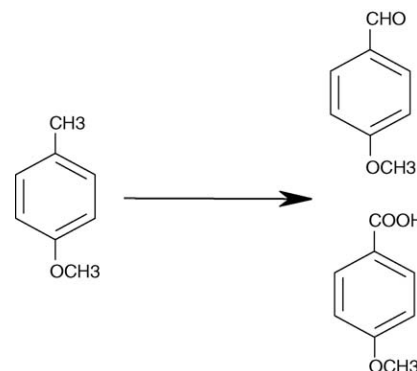


Benjaram M. Reddy, Komateedi N. Rao, Gunugunuri K. Reddy, Pankaj Bharali

Journal of Molecular Catalysis A: Chemical 253 (2006) 44

Characterization and catalytic activity of V₂O₅/Al₂O₃-TiO₂ for selective oxidation of 4-methylanisole

The Al₂O₃-TiO₂ support accommodates a monolayer equivalent of V₂O₅ in a highly dispersed state and exhibits good catalytic activity for oxidation of 4-methylanisole to *p*-anisaldehyde and *p*-anisic acid in vapour phase under normal atmospheric pressure. These catalysts were characterized by means of XRD, FTIR, XPS, O₂ chemisorption and BET surface area methods to correlate with catalytic properties.

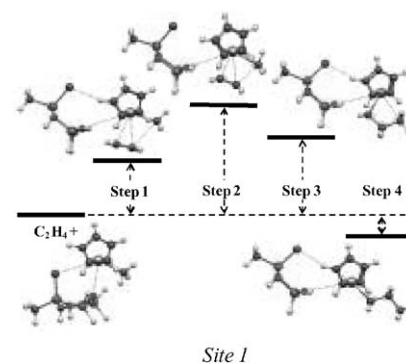


P.G. Belelli, N.J. Castellani

Journal of Molecular Catalysis A: Chemical 253 (2006) 52

Counterion and additive effects on ethylene coordination and insertion in metallocene catalyst

A theoretical analysis of coordination and insertion of ethylene molecule on different metallocenic active sites were performed. The influence of the counterion on the energy barrier that the olefin must overcome for its coordination and insertion was considered. The presence of the AlCl_3 additive reduces the maximum energy and improves the stability of the final propyl ionic-pair.

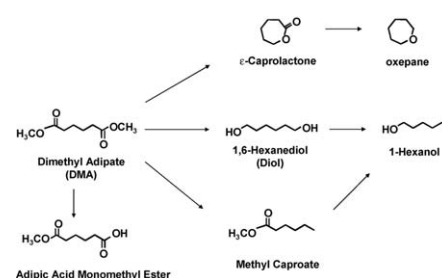


Adriana M. Silva, Onélia A.A. Santos, Marco A. Morales, Elisa M. Baggio-Saitovitch, Elizabete Jordão, Marco A. Fraga

Journal of Molecular Catalysis A: Chemical 253 (2006) 62

Role of catalyst preparation on determining selective sites for hydrogenation of dimethyl adipate over $\text{RuSn}/\text{Al}_2\text{O}_3$

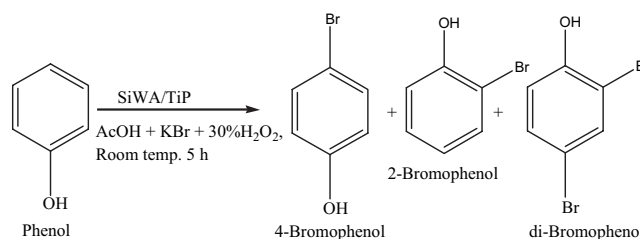
The effects of the preparation method and pretreatment conditions on the selective production of 1,6-hexanediol was studied. The catalysts were prepared by co-impregnation and sol gel methods. The results presented in this work indicated that alumina-supported Ru–Sn bimetallic catalysts may be appropriate for 1,6-hexanediol production from DMA. The generation of tin oxidic species is not solely decisive for the formation of catalytically active sites. A suitable preparation method must be applied in order to better localize the SnO_x moieties and tailor the required Ru– SnO_x selective sites as revealed by XPS and Mössbauer spectroscopy.

**D.P. Das, K.M. Parida**

Journal of Molecular Catalysis A: Chemical 253 (2006) 70

Liquid phase bromination of phenol
III. Over heteropoly acid (HPA)-impregnated titanium phosphate (TiP)

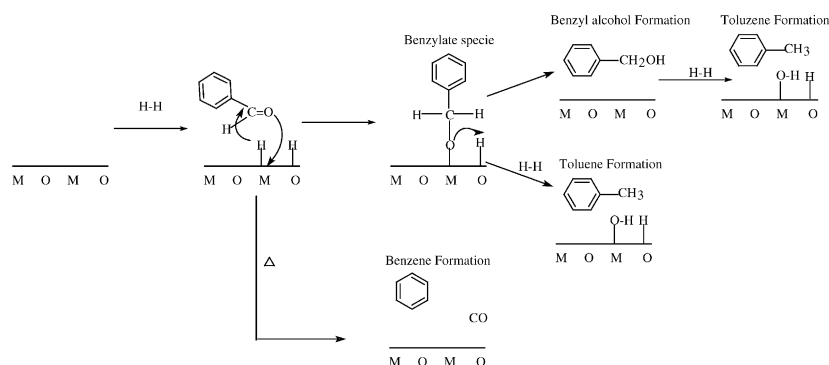
Among the entire HPA-impregnated TiP series, PWA/TiP has got the highest acidic character (130.3 $\mu\text{mol/g}$). Even so SiWA/TiP, dried at 110 °C showed the highest *para*-selectivity (30%). With increase in the activation temperature up to 400 °C for 15 wt.% SiWA/TiP, the *para*-selectivity (4-BP/2-BP) goes on increasing from 0.26 to 1.85 due to the increase in the Lewis acidic character and thereafter the value remains constant. Similarly with increase in the reaction time (h) and catalyst concentration (g/mol), the selectivity ratio (4-BP/2-BP) increases from 1.05 to 1.85 and from 1.23 to 1.85, respectively



A. Saadi, R. Merabti, Z. Rassoul, M.M. Bettahar

Journal of Molecular Catalysis A: Chemical 253 (2006) 79

Benzaldehyde hydrogenation over supported nickel catalysts

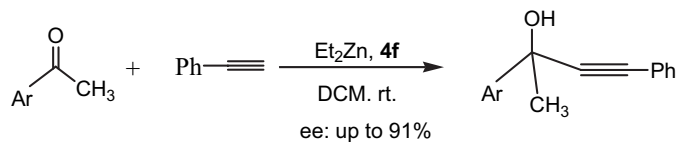


**Hua-qing Cai, Chao Chen, Lei Liu,
Jing-man Ni, Rui Wang**

Journal of Molecular Catalysis A: Chemical 253
(2006) 86

A new type of ligand derived from N-terminal protected dipeptides in enantioselective addition of phenylacetylene to aromatic ketones at room temperature

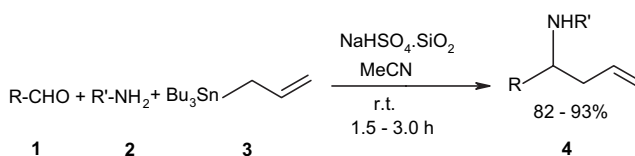
A new type of ligand derived from N-terminal protected L-Phe-based dipeptides was found to be effective in catalyzing the enantioselective addition of phenylacetylene to aromatic ketones with up to 91% ee. The reaction required no other metal to promote than Et_2Zn . The whole process was completed at room temperature and proceeded under very mild reaction conditions.



**Biswanath Das, B. Ravikanth,
K. Laxminarayana, B. Vittal Rao**

Journal of Molecular Catalysis A: Chemical 253
(2006) 92

A simple and facile synthesis of homoallylic amines using silica supported sodium hydrogen sulfate

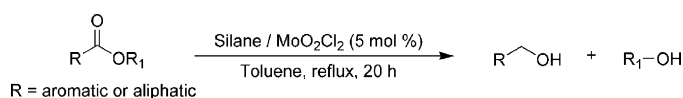


Ana C. Fernandes, Carlos C. Romão

Journal of Molecular Catalysis A: Chemical 253
(2006) 96

Silane/ MoO_2Cl_2 as an efficient system for the reduction of esters

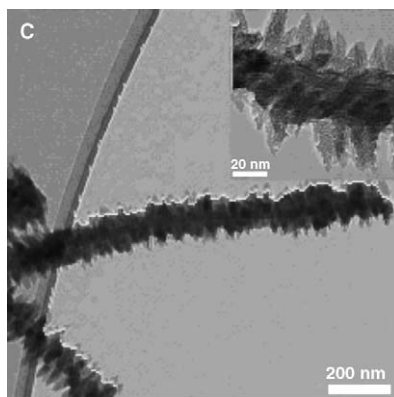
The system silane/ MoO_2Cl_2 (5 mol%) proved to be very efficient for the reduction of aliphatic and aromatic esters to the corresponding alcohols in good yields.



Huogen Yu, Jiaguo Yu, Bei Cheng

Journal of Molecular Catalysis A: Chemical 253
(2006) 99

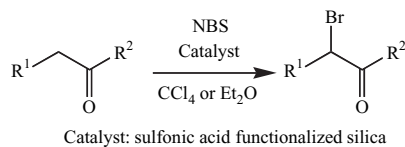
Preparation, characterization and photocatalytic activity of novel TiO_2 nanoparticle-coated titanate nanorods



**Biswanath Das, Katta Venkateswarlu,
Harish Holla, Maddeboina Krishnaiah**

Journal of Molecular Catalysis A: Chemical 253
(2006) 107

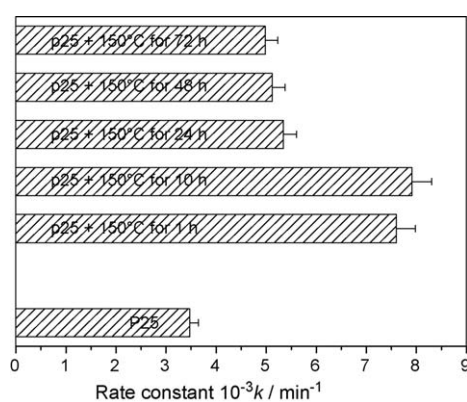
Sulfonic acid functionalized silica: A remarkably efficient heterogeneous reusable catalyst for α -monobromination of carbonyl compounds using *N*-bromosuccinimide



**Jiaguo Yu, Huogen Yu, Bei Cheng,
Minghua Zhou, Xiujian Zhao**

Journal of Molecular Catalysis A: Chemical 253
(2006) 112

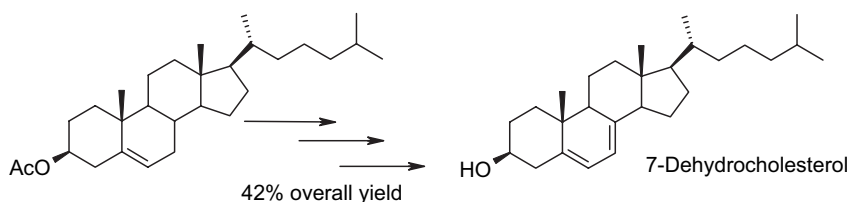
Enhanced photocatalytic activity of TiO₂ powder (P25) by hydrothermal treatment



Diane Dugas, Jean Michel Brunel

Journal of Molecular Catalysis A: Chemical 253
(2006) 119

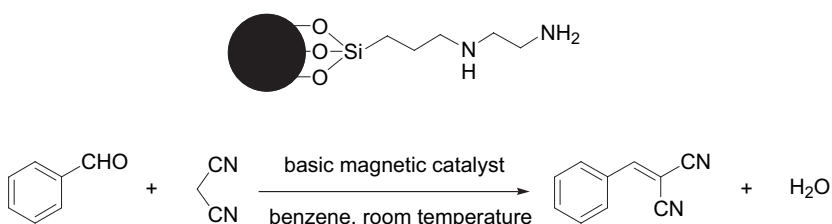
Synthesis of 7-dehydrocholesterol through a palladium catalyzed selective homoannular conjugated diene formation



Nam T.S. Phan, Christopher W. Jones

Journal of Molecular Catalysis A: Chemical 253
(2006) 123

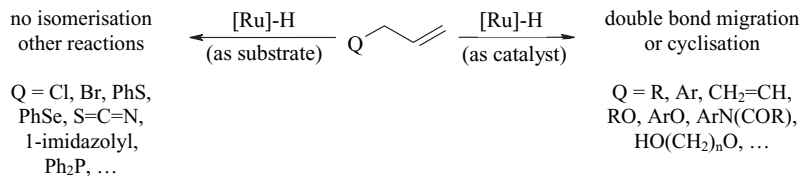
Highly accessible catalytic sites on recyclable organosilane-functionalized magnetic nanoparticles: An alternative to functionalized porous silica catalysts



**S. Krompiec, N. Kuźnik, M. Krompiec,
R. Penczek, J. Mrzığod, A. Tórz**

Journal of Molecular Catalysis A: Chemical 253
(2006) 132

The role of the functional group in double bond migration in allylic systems catalysed by ruthenium hydride complexes

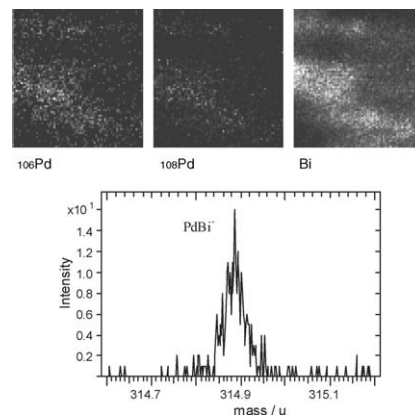


S. Karski

Journal of Molecular Catalysis A: Chemical 253
(2006) 147

Activity and selectivity of Pd–Bi/SiO₂ catalysts in the light of mutual interaction between Pd and Bi

The presence of intermetallic compounds on the surface of 5% Pd–5% Bi/SiO₂ catalysts are confirmed by ToF-SIMS measurements. The studies reveal lack of homogeneity of the sample. Palladium and bismuth are found in distinct clusters on the studied area, and so they are not evenly dispersed on the carrier. The concentration of palladium and bismuth is the highest on the same areas of the studied sample. Moreover, in the spectrum of secondary ions maxima of signal intensity for the following mass: 314, 315 and 317 ascribed to intermetallic compound BiPd were found.

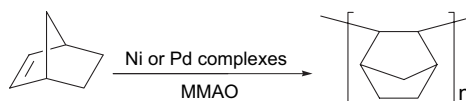


**Tao Hu, Yan-Guo Li, Yue-Sheng Li,
Ning-Hai Hu**

Journal of Molecular Catalysis A: Chemical 253
(2006) 155

Novel highly active binuclear neutral nickel and palladium complexes as precatalysts for norbornene polymerization

A series of binuclear neutral nickel and palladium complexes [(XC₆H₄CH=NC₆H₃-iPr₂)MRL]₂ **4b–f** (X = H or NO₂, M = Ni or Pd, R = Ph or Me, L = PPh₃ or Py) and [(C₁₀H₇CH=NC₆H₃-iPr₂)MRL]₂ **8a–c** (M = Ni or Pd, R = Ph or Me, L = PPh₃ or Py) have been synthesized and characterized, and were shown to be highly active catalysts for vinylic polymerization of norbornene.

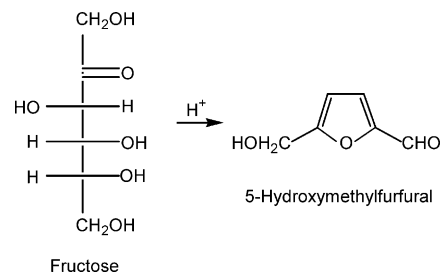


Claude Moreau, Annie Finiels, Laurent Vanoye

Journal of Molecular Catalysis A: Chemical 253
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Dehydration of fructose and sucrose into 5-hydroxymethylfurfural in the presence of 1-H-3-methyl imidazolium chloride acting both as solvent and catalyst

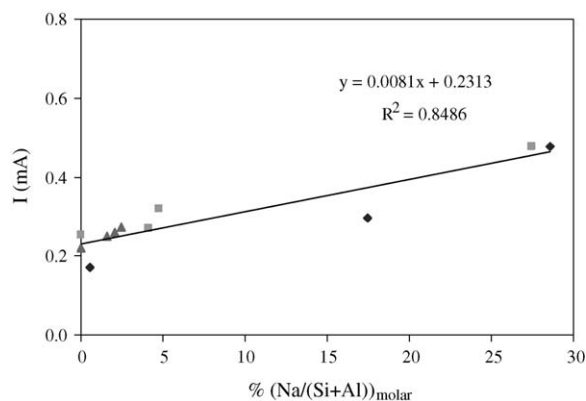
The commercially available ionic liquid 1-H-3-methyl imidazolium chloride catalyzes the dehydration of fructose and sucrose into 5-hydroxymethylfurfural in a nearly quantitative yield, at low temperature, short reaction time and relatively facile extraction of the final product and ionic liquid recycling.



**R.H. Carvalho, M.A.N.D.A. Lemos, F. Lemos,
J.M.S. Cabral, F. Ram6a Ribeiro**

Journal of Molecular Catalysis A: Chemical 253
(2006) 170

Electro-oxidation of phenol on zeolite/graphite
composite electrodes
Part 2. Influence of zeolite type and composition

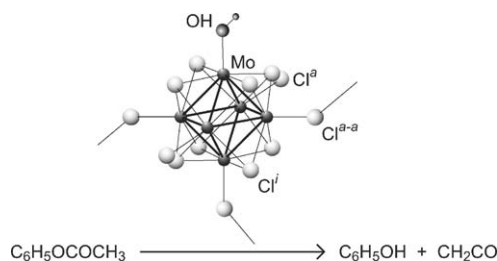


**Satoshi Kamiguchi, Takashi Mori,
Masaki Watanabe, Akane Suzuki,
Mitsuo Kodomari, Masaharu Nomura,
Yasuhiro Iwasawa, Teiji Chihara**

Journal of Molecular Catalysis A: Chemical 253
(2006) 176

Retention of the octahedral metal framework of Nb
and Mo halide clusters in catalytic decomposition of
phenyl acetate to phenol and ketene

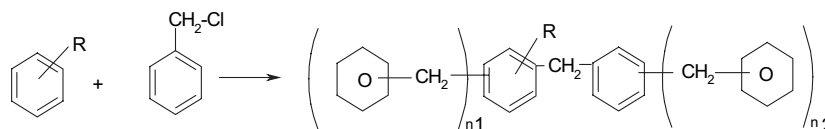
When molecular halide clusters $[(\text{Nb}_6\text{Cl}_{12})\text{Cl}_2(\text{H}_2\text{O})_4]\cdot 4\text{H}_2\text{O}$ and $(\text{H}_3\text{O})_2[(\text{Mo}_6\text{Cl}_8)\text{Cl}_6]\cdot 6\text{H}_2\text{O}$ were treated in a helium stream at 250 °C and 400 °C, respectively, the maximum catalytic activities for decomposition of phenyl acetate to phenol and ketene appeared. The activity was ascribed to the Brønsted acidity of the hydroxo ligand formed, and the retention of the octahedral cluster frameworks was ascertained.



K. Bachari, O. Cherifi

Journal of Molecular Catalysis A: Chemical 253
(2006) 187

Gallium-containing mesoporous silicas as a catalyst
for alkylation of benzene and other aromatics by
benzyl chloride

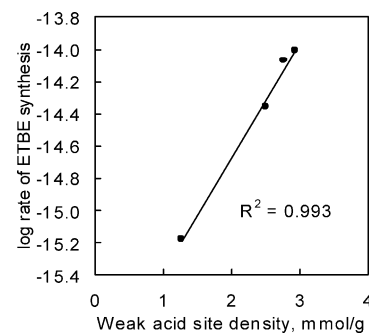


N.V. Vlasenko, Yu.N. Kochkin, A.M. Puziy

Journal of Molecular Catalysis A: Chemical 253
(2006) 192

Liquid phase synthesis of ethyl-*tert*-butyl ether: The
relationship between acid, adsorption and catalytic
properties of zeolite catalysts

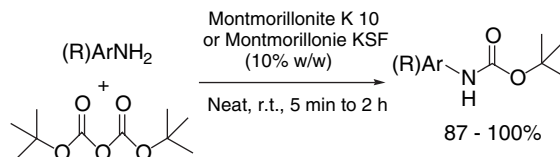
The role of acid centers of natural zeolites in ethyl-*tert*-butyl ether (ETBE) synthesis was investigated. An approach for calculation of desorption energy distribution from stepwise desorption experiment was proposed. The correlation between the rate of ETBE synthesis and concentration of weak acid sites ($E_{\text{NH}_3} = 70\text{--}75$ kJ/mol) was found (see figure). Active in ETBE synthesis are low energy surface ethanol complexes ($E_{\text{C}_2\text{H}_5\text{OH}} = 53\text{--}60$ kJ/mol), which are located on weak acid centers of zeolites.



Sunay V. Chankeshwara, Asit K. Chakraborti

Journal of Molecular Catalysis A: Chemical 253 (2006) 198

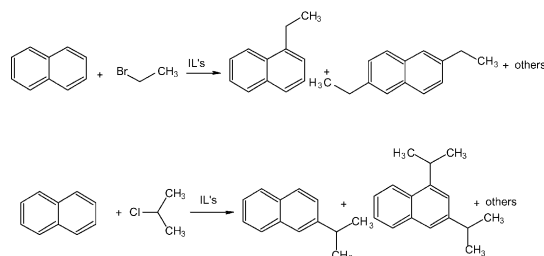
Montmorillonite K 10 and montmorillonite KSF as new and reusable catalysts for conversion of amines to *N*-*tert*-butylcarbamates


Carlos Gutierrez Blanco, Dolores Casal Banciella, M. Dolores González Azpíroz

Journal of Molecular Catalysis A: Chemical 253 (2006) 203

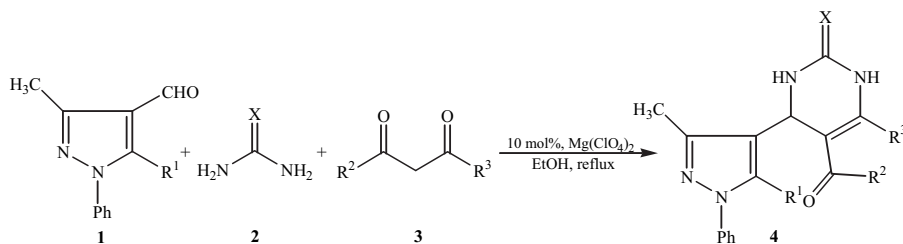
Alkylation of naphthalene using three different ionic liquids

Three ionic liquid systems were used as reaction media for the alkylation of naphthalene with different reagents. The following cations were used to prepare the chloroaluminate(III) ionic liquids: 1-butyl-3-methylimidazolium; 8-butyl-1,8-diazabicyclo[5,4,0]undec-7-enium and 5-butyl-1,5-diazabicyclo[4,3,0]-non-5-enium. The conversions and reaction yields produced by the alkylation reaction of naphthalene with ethylbromide and isopropylchloride in the three ionic liquid systems were compared.


Xinli Zhang, Yanping Li, Chenjiang Liu, Jide Wang

Journal of Molecular Catalysis A: Chemical 253 (2006) 207

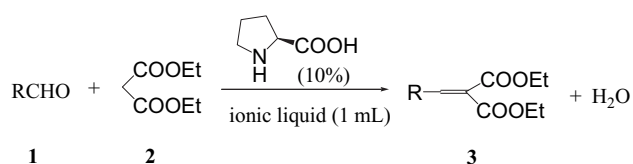
An efficient synthesis of 4-substituted pyrazolyl-3,4-dihydropyrimidin-2(1H)-(thio)ones catalyzed by $Mg(ClO_4)_2$ under ultrasound irradiation


Yun Wang, Zhi-cai Shang, Tian-xing Wu, Ji-cai Fan, Xiang Chen

Journal of Molecular Catalysis A: Chemical 253 (2006) 212

Synthetic and theoretical study on proline-catalyzed Knoevenagel condensation in ionic liquid

A novel and highly efficient method for Knoevenagel condensation using *L*-proline as catalyst and ionic liquid as green solvent is described. In addition, the results of calculations with the Gaussian 98 suite of program are in good accordance with the experimental outcomes.

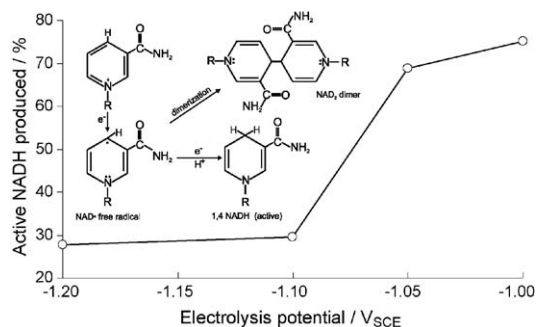


Alexis Damian, Sasha Omanovic

Journal of Molecular Catalysis A: Chemical 253 (2006) 222

Electrochemical reduction of NAD^+ on a polycrystalline gold electrode

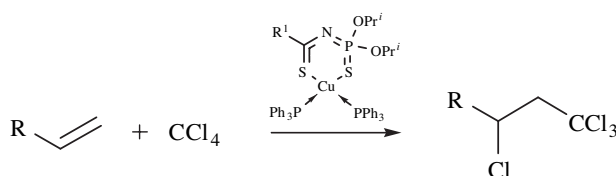
The reduction of NAD^+ on a gold electrode results in the formation of two products: enzymatically active 1,4-NADH and inactive NAD_2 . The ratio between the two products formed is highly potential dependent.



**Alexey Zazybin, Olga Osipova,
Ulya Khusnutdinova, Ilya Aristov,
Boris Solomonov, Felix Sokolov,
Maria Babashkina, Nail Zabiroy**

Journal of Molecular Catalysis A: Chemical 253 (2006) 234

Addition of tetrachloromethane to alkenes catalyzed by copper(I) complexes with *N*-thioacylamidothio-phosphate ligands

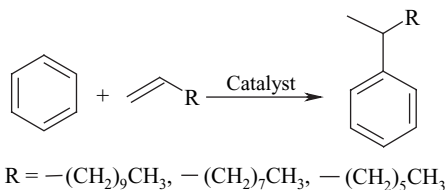


**Ankur Bordoloi, Biju M. Devassy,
P.S. Niphadkar, P.N. Joshi, S.B. Halligudi**

Journal of Molecular Catalysis A: Chemical 253 (2006) 239

Shape selective synthesis of long-chain linear alkyl benzene (LAB) with AIMCM-41/Beta zeolite composite catalyst

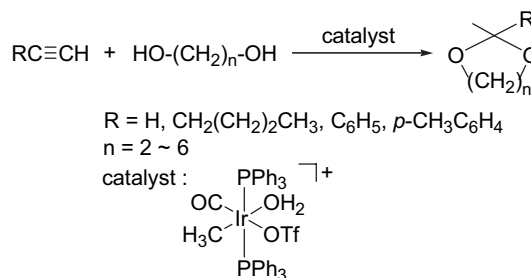
AIMCM-41/Beta zeolite composite catalyst was prepared by seeding method using Beta zeolite as a seed and tested in the liquid-phase synthesis of long-chain linear alkyl benzenes. Under the reaction conditions of 120 °C, benzene/1-dodecene molar ratio 10 and time 2 h, conversion of dodecene was 48% with 2-dodecylbenzene selectivity 76%.

**Song yi Kim, Chong Shik Chin, Min-Sik Eum**

Journal of Molecular Catalysis A: Chemical 253 (2006) 245

Cyclic acetals from catalytic addition of diols to terminal alkynes with a cationic iridium complex containing two labile ligands

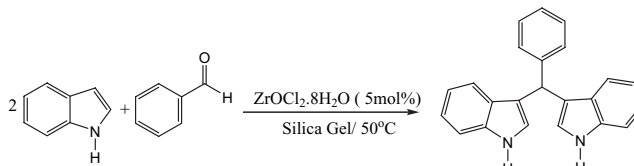
Cationic iridium complex $[\text{Ir}(\text{CH}_3)(\text{OTf})(\text{CO})(\text{OH}_2)(\text{PPh}_3)_2](\text{OTf})$ catalyzes addition of diols ($\text{HO}-(\text{CH}_2)_n-\text{OH}$ ($n = 2-6$)) to terminal alkynes ($\text{RC}\equiv\text{CH}$; $\text{R} = \text{H}, \text{CH}_2(\text{CH}_2)_2\text{CH}_3, \text{C}_6\text{H}_5, p\text{-CH}_3\text{C}_6\text{H}_4$) to produce cyclic acetals $\text{CH}_3\text{C}(\text{R})\text{O}(\text{CH}_2)_n\text{O}$ exclusively in the absence of H_2O at room temperature.



**Habib Firouzabadi, Nasser Iranpoor,
Maasoumeh Jafarpour, Arash Ghaderi**

Journal of Molecular Catalysis A: Chemical 253
(2006) 249

ZrOCl₂•8H₂O/silica gel as a new efficient and a highly water-tolerant catalyst system for facile condensation of indoles with carbonyl compounds under solvent-free conditions

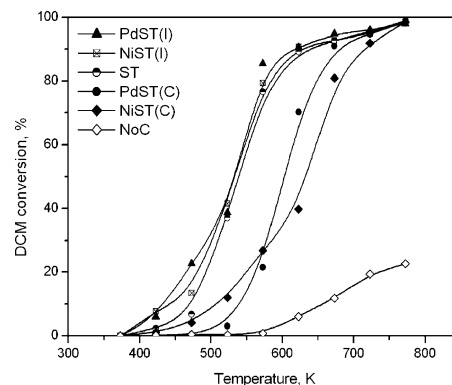


**L.M. Martínez T, C. Montes de Correa,
J.A. Odriozola, M.A. Centeno**

Journal of Molecular Catalysis A: Chemical 253
(2006) 252

Synthesis and characterization of xerogel titania modified with Pd and Ni

Bifunctional catalysts, i.e. containing palladium and Brønsted acid sites are required for total combustion of dichloromethane (DCM) at relatively low temperatures. DCM oxidation is much higher over sulphated catalysts as compared to un-sulphated ones, catalysts prepared by impregnation exhibit higher activity than those prepared by cogellation and Pd was more effective than Ni for burning-off coke deposited over support surface.

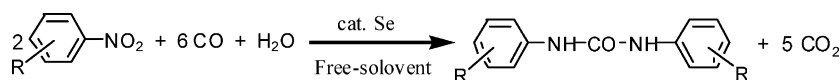


**Xiaofang Wang, Peng Li, Xiaohua Yuan,
Shiwei Lu**

Journal of Molecular Catalysis A: Chemical 253
(2006) 261

Selenium-catalyzed carbonylation of nitroarenes to symmetrical 1,3-diarylureas under solvent-free conditions

Diarylureas were synthesized by Se-catalyzed carbonylation of nitroarenes in up to 98% yields. Additionally, three herbicides were readily produced from diarylureas and amine.

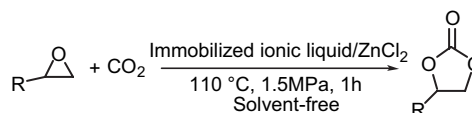


**Lin-Fei Xiao, Fu-Wei Li, Jia-Jian Peng,
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Journal of Molecular Catalysis A: Chemical 253
(2006) 265

Immobilized ionic liquid/zinc chloride: Heterogeneous catalyst for synthesis of cyclic carbonates from carbon dioxide and epoxides

Chemical fixation of carbon dioxide with epoxides to form cyclic carbonates proceeds very effectively under mild conditions by using immobilized ionic liquid catalyst in conjunction with zinc chloride without any organic solvents. Reaction temperature, carbon dioxide pressure, effects of different metallic complexes and the amount of immobilized ionic liquid were investigated. The optimum reaction conditions were 110 °C and 1.5 MPa, and the catalyst system was recycled and reused.

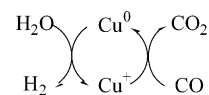


**Tetsuya Shishido, Manabu Yamamoto,
Ikuo Atake, Dalin Li, Yan Tian,
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Tsuneji Sano, Katsuomi Takehira**

Journal of Molecular Catalysis A: Chemical 253
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Cu/Zn-based catalysts improved by adding
magnesium for water–gas shift reaction

Cu/MgO/ZnO catalyst prepared by homogeneous precipitation showed high catalytic activity for water–gas shift reaction. Small amount of MgO enhanced and stabilized the formation of Cu⁺ species, resulting in the high activity. The reaction proceeds via a reduction–oxidation mechanism between Cu⁺ and Cu⁰ on the catalyst surface.



**Tomonori Kawabata, Naoko Fujisaki,
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Journal of Molecular Catalysis A: Chemical 253
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Improved Fe/Mg–Al hydrotalcite catalyst for
Baeyer–Villiger oxidation of ketones with molecular
oxygen and benzaldehyde

Fe/Mg₃Al prepared by the ‘memory effect’ exhibited a high catalytic activity for Baeyer–Villiger oxidation of ketones using molecular oxygen and benzaldehyde. The Fe/Mg₃Al catalyst showed higher activity than that prepared by coprecipitation, and the prominent catalytic performance could be ascribed to cluster-like octahedrally coordinated Fe³⁺ species incorporated on the surface of Mg–Al mixed oxide.

