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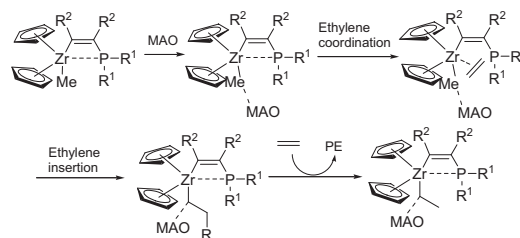
Articles

Peng Hao, Shu Zhang, Jianjun Yi, Wen-Hua Sun

Journal of Molecular Catalysis A: Chemical 302 (2009) 1

Zirconadihydrophosphetes as highly active species for ethylene polymerization

A series of zirconoalkenylphosphines were synthesized as the highly active catalysts for ethylene polymerization and copolymerization with α -olefins or norbornene in presence of MAO. The possible mechanism in polymerization was provided according to ethylene activation experiment and data from ^1H , ^{13}C and ^{31}P NMR.

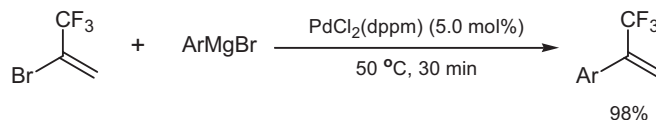


Osamu Kobayashi, Daisuke Uraguchi, Tetsu Yamakawa

Journal of Molecular Catalysis A: Chemical 302 (2009) 7

Synthesis of α -trifluoromethylstyrene derivatives via Pd-catalyzed cross-coupling of 2-bromo-3,3,3-trifluoropropene and arylmagnesium bromides

The Pd-catalyzed cross-coupling of 2-bromo-3,3,3-trifluoropropene and arylmagnesium bromides was investigated. $\text{PdCl}_2(\text{dppm})$ gave the highest yield of α -trifluoromethylstyrene (98%) from 2-bromo-3,3,3-trifluoropropene and phenylmagnesium bromide in 1,4-dioxane solvent. This $\text{PdCl}_2(\text{dppm})$ -catalyzed coupling could be applied to the synthesis of α -trifluoromethylstyrene derivatives in satisfactory yields using some arylmagnesium bromides.

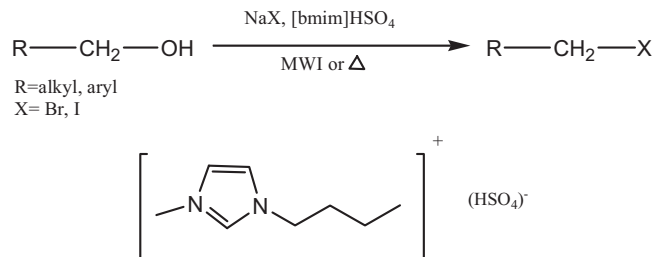


Neeraj Gupta, Goverdhan L. Kad, Jasvinder Singh

Journal of Molecular Catalysis A: Chemical 302 (2009) 11

Enhancing nucleophilicity in ionic liquid [bmim]HSO₄: A recyclable media and catalyst for the halogenation of alcohols

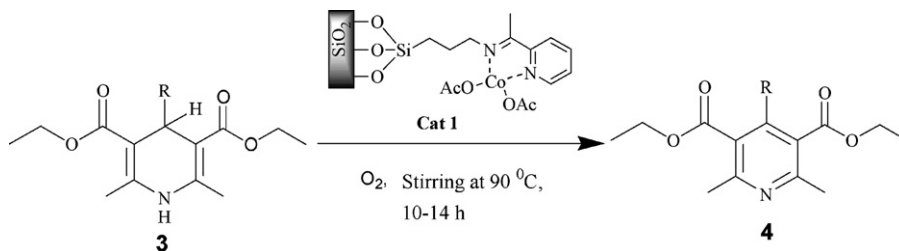
Ionic liquid 1-butyl-3-methylimidazolium hydrogen sulphate [bmim]HSO₄ has been demonstrated as an efficient reusable catalyst and solvent, for the halogenation of aromatic and aliphatic alcohols with alkali metal salts (NaBr, NaI) in conjunction with microwave and thermal heating.



Tahira Shamim, Monika Gupta, Satya Paul*Journal of Molecular Catalysis A: Chemical* 302 (2009) 15

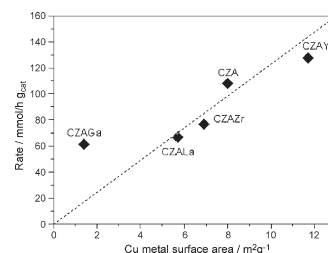
The oxidative aromatization of Hantzsch 1,4-dihydropyridines by molecular oxygen using surface functionalized silica supported cobalt catalysts

The oxidative aromatization of Hantzsch 1,4-dihydropyridines to the corresponding pyridines with molecular oxygen as oxidant is catalyzed by covalently anchored cobalt complexes onto the surface of silica gel. Cat **1** was found to be the most effective and stable under the reaction conditions. It can be easily recovered and recycled.

**Akula Venugopal, Jelliarko Palgunadi, Jung Kwang Deog, Oh-Shim Joo, Chae-Ho Shin***Journal of Molecular Catalysis A: Chemical* 302 (2009) 20

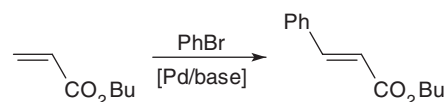
Dimethyl ether synthesis on the admixed catalysts of Cu-Zn-Al-M (M = Ga, La, Y, Zr) and $\gamma-Al_2O_3$: The role of modifier

Dimethyl ether synthesis on the admixed catalysts of Cu-based and solid acid catalysts has been examined. The yttrium-modified Cu-Zn-Al admixed with $\gamma-Al_2O_3$ is superior in activity with a DME yield of 47.7% to other Cu-based catalysts. This high activity is attributed to the increase in Cu metal surface area by the addition of yttrium.

**Jan Demel Sujandi, Sang-Eon Park, Jiří Čejka, Petr Štěpnička***Journal of Molecular Catalysis A: Chemical* 302 (2009) 28

Preparation of heterogeneous catalysts supported on mesoporous molecular sieves modified with various N-groups and their use in the Heck reaction

Catalytic performance of supported catalysts obtained from mesoporous molecular sieves modified with N-donor groups and palladium(II) acetate in the Heck coupling is controlled by the modifying group. The most efficient catalyst possessing $=SiCH_2CH_2CH_2NH_2$ and $=SiCH_2CH_2CH_2NHCH_2CH_2NEt_2$ groups afforded the coupling product in conversion as high as 90% under microwave irradiation for 30 min and up to 84% under solvothermal conditions ($160\ ^\circ C/4\ h$) when combined with sodium acetate. The latter catalyst also displayed considerable bifunctional (i.e., metal-containing and basic) character.

**Ajaya Kumar Singh, Reena Negi, Yokraj Katre, Surya Prakash Singh***Journal of Molecular Catalysis A: Chemical* 302 (2009) 36

Mechanistic study of novel oxidation of paracetamol by chloramine-T using micro-amount of chloro-complex of Ir(III) as a homogeneous catalyst in acidic medium

The following rate law is proposed for the mechanistic study of novel oxidation of paracetamol by chloramine-T using micro-amount of chloro-complex of Ir(III) as a homogeneous catalyst in acidic medium to explain the observed experimental results.

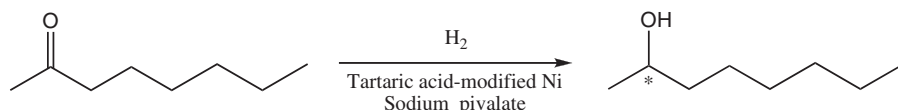
$$\text{rate} = \frac{2kK_1K_2K_3K_4[\text{CAT}][\text{Cl}][\text{PA}][\text{Ir(III)}]_T}{[\text{H}^+][\text{TsNH}_2] + K_2[\text{H}^+][\text{TsNH}_2][\text{Cl}^-] + K_3K_2[\text{PA}][\text{Cl}^-][\text{H}^+][\text{TsNH}_2] + K_1K_2K_3K_4[\text{CAT}][\text{PA}][\text{Cl}^-]}$$

Tsutomu Osawa, Yuki Nakagawa, Masashi Ando, Tadao Harada, Osamu Takayasu

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Studies of co-modifier and carboxylic acid for the enantio-differentiating hydrogenation of 2-octanone over a tartaric acid in situ modified nickel catalyst

The effects of a co-modifier and carboxylic acid on the hydrogenation rate and the enantio-differentiating ability (e.d.a.) were studied for the hydrogenation of 2-octanone over a tartaric acid modified reduced nickel catalyst. Sodium pivalate, instead of the typical co-modifier, NaBr, was appropriate for the in situ modification of reduced nickel. The use of sodium pivalate resulted in a higher hydrogenation rate and e.d.a.

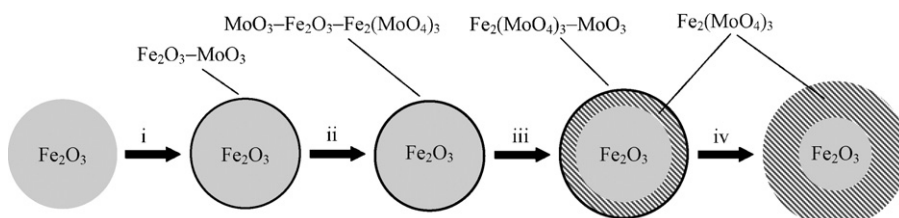


Yan Huang, Liyan Cong, Jian Yu, Pierre Eloy, Patricio Ruiz

Journal of Molecular Catalysis A: Chemical 302 (2009) 48

The surface evolution of a catalyst jointly influenced by thermal spreading and solid-state reaction: A case study with an Fe_2O_3 - MoO_3 system

Mixed oxides are a particularly important group of catalytic materials, and it is of great interest to investigate the evolution of the surface state during the preparation of a catalyst. This work studied Fe_2O_3 - MoO_3 as a model system, investigating the surface states jointly influenced by the thermal spreading of MoO_3 and the solid-state reaction that produces $\text{Fe}_2(\text{MoO}_4)_3$ during heat treatment.

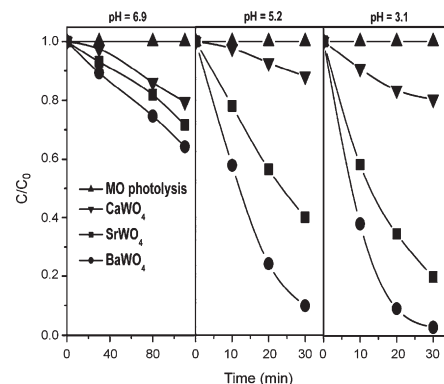


Zhichao Shan, Yaoming Wang, Hanming Ding, Fuqiang Huang

Journal of Molecular Catalysis A: Chemical 302 (2009) 54

Structure-dependent photocatalytic activities of MWO_4 ($M = \text{Ca}, \text{Sr}, \text{Ba}$)

The isostructural photocatalysts MWO_4 ($M = \text{Ca}, \text{Sr}, \text{Ba}$) were synthesized by a solid state reaction, were investigated. The photocatalytic activity for decomposing methyl orange is in the increasing order of $\text{CaWO}_4 < \text{SrWO}_4 < \text{BaWO}_4$ under both neutral and acidic conditions. The investigation indicates that the lower packing factor, leads to the better photocatalytic activity.

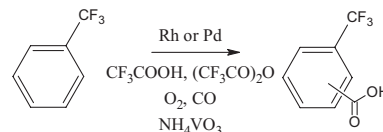


Joseph Zakzeski, Alexis T. Bell

Journal of Molecular Catalysis A: Chemical 302 (2009) 59

Oxidative carbonylation of benzotrifluoride to form trifluoromethylbenzoic acid

The oxidative carbonylation of benzotrifluoride to form trifluoromethylbenzoic acid (TFMBA) has been catalyzed using either Rh(III) or a Pd(II) cation in combination with a carboxylic acid and its anhydride, ammonium metavanadate, CO, and O_2 . The influence of metal cation and vanadate concentrations, temperature, time, acid composition, and gas pressures, were explored.

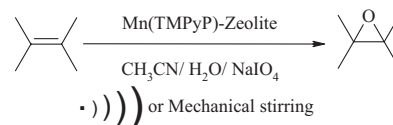


Majid Moghadam, Shahram Tangestaninejad, Valiollah Mirkhani, Iraj Mohammadpoor-Baltork, Maryam Moosavifar

Journal of Molecular Catalysis A: Chemical 302 (2009) 68

Host (nanocavity of zeolite-Y or X)-guest (manganese (III) tetrakis[4-N-methylpyridinium]porphyrin) nanocomposite materials as efficient catalysts for biomimetic alkene epoxidation with sodium periodate: Shape-selective epoxidation of linear alkenes

Manganese (III) 5,10,15,20-tetrakis(4-N-methylpyridyl) porphyrin encapsulated into zeolite X and zeolite Y was synthesized and used as catalysts for epoxidation of cyclic and linear alkenes with NaIO_4 under mechanical stirring and ultrasonic irradiation. These catalysts were also used for epoxidation of linear alkenes and good shape selectivity was observed.

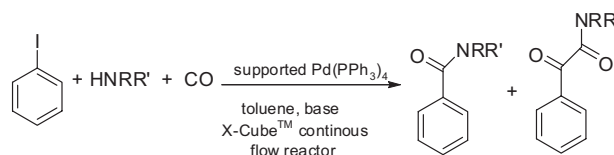


János Balogh, Árpád Kuik, László Úrge, Ferenc Darvas, József Bakos, Rita Skoda-Földes

Journal of Molecular Catalysis A: Chemical 302 (2009) 76

Double carbonylation of iodobenzene in a microfluidics-based high throughput flow reactor

Double carbonylation of iodobenzene in the presence of amines were carried out effectively in a microfluidics-based flow reactor (X-Cube™) of high throughput capability using immobilized $\text{Pd}(\text{PPh}_3)_4$ catalyst. By the proper tuning of the reaction conditions α -ketoamides could be synthesized with 70–96% selectivities depending on the choice of the nucleophile. The highest yields of double carbonylation products were obtained at relatively low temperature (80 °C) and using DBU as the base with primary amines as the reaction partners. Imine formation was observed only at higher temperatures.

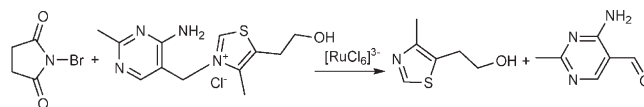


K.N. Mohana, K.R. Ramya

Journal of Molecular Catalysis A: Chemical 302 (2009) 80

Ruthenium (III)-catalyzed oxidative cleavage of thiamine hydrochloride with N-bromosuccinimide in presence of hydrochloric acid medium: A kinetic and mechanistic approach

The kinetics of ruthenium (III)-catalyzed oxidative cleavage of thiamine hydrochloride (THM) with N-bromosuccinimide in HCl medium has been studied. The reaction follows the rate law, $-d[\text{NBS}]/dt = k[\text{NBS}]^a [\text{Ru(III)}]^b [\text{THM}]^c [\text{H}^+]^{-c} [\text{Cl}^-]^{-d}$, where a , b , c and d are less than unity. The stoichiometry of the reaction was found to be 1:1, and the oxidation products were identified.

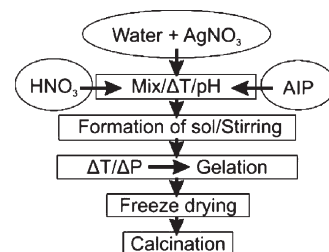


Hannes Kannisto, Hanna Härelind Ingelsten, Magnus Skoglundh

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Ag-Al₂O₃ catalysts for lean NO_x reduction—Influence of preparation method and reductant

Ag-Al₂O₃ samples were prepared via impregnation (I) and two sol-gel routes, including thermal drying (II) or freeze-drying (III, not previously reported). Characterization confirmed sol-gel samples containing more dispersed silver than corresponding impregnated samples. Silver clusters were indicated in samples by routes (I) and (II). A crucial ratio between oxidized silver species and clusters for high NO_x reduction is implied.

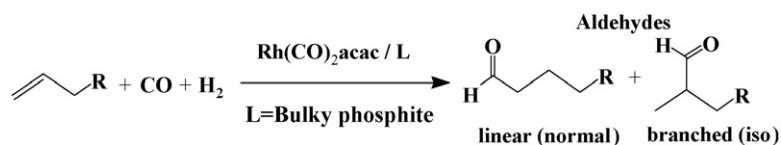


Aasif A. Dabbawala, Hari C. Bajaj, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 302 (2009) 97

Rhodium complex of monodentate phosphite as a catalyst for olefins hydroformylation

A novel monodentate bulky phosphite ligand, tri-1-naphthylphosphite (TNPST) has been synthesized and characterized. The catalytic performance of its Rhodium complex is investigated for the hydroformylation of dissimilar alkenes specifically 1-hexene, styrene, and cyclohexene. The steric attributes of free ligand is investigated by cone angle method.

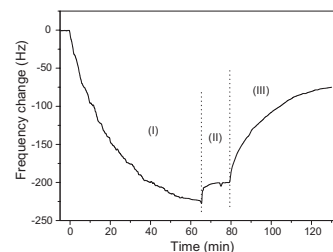


Zhengpeng Yang, Chunjing Zhang

Journal of Molecular Catalysis A: Chemical 302 (2009) 107

Adsorption and photocatalytic degradation of bilirubin on hydroxyapatite coatings with nanostructural surface

The frequency change of quartz crystal microbalance with time in the process of adsorption and photocatalytic degradation of bilirubin on hydroxyapatite coatings with nanostructural surface. (I) bilirubin adsorption, (II) rinsing with DI water, (III) degradation of bilirubin during UV illumination.

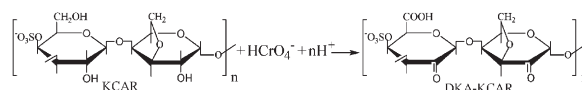


I.A. Zaafarany, K.S. Khairou, R.M. Hassan

Journal of Molecular Catalysis A: Chemical 302 (2009) 112

Acid-catalysis of chromic acid oxidation of kappa-carrageenan polysaccharide in aqueous perchlorate solutions

The kinetics of oxidation of kappa-carrageenan (KCAR) polysaccharide by chromic acid in aqueous perchlorate solutions have been investigated spectrophotometrically. A kinetic evidence for the formation of 1:2 intermediate complex is revealed. The oxidation product was identified by the spectral data and microanalysis as diketo-acid derivative (DKA-KCAR).

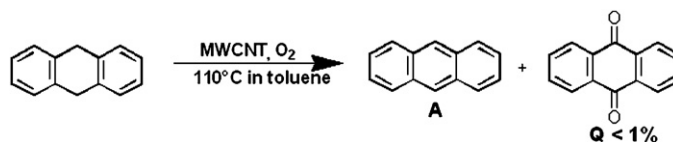


Dominique Bégin, Gilles Ulrich, Julien Amadou, Dang Sheng Su, Cuong Pham-Huu, Raymond Ziesel

Journal of Molecular Catalysis A: Chemical 302 (2009) 119

Oxidative dehydrogenation of 9,10-dihydroanthracene using multi-walled carbon nanotubes

Multi-walled carbon nanotubes promote oxidative dehydrogenation of 9,10-dihydroanthracene in the absence of trace amounts of metals. Thermal treatment of the carbon nanostructure improves the catalytic activity versus charcoal or exfoliated carbon.

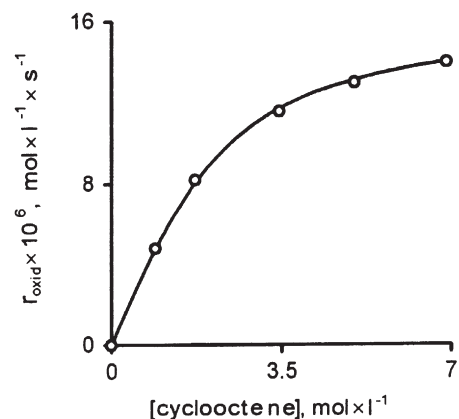


**Yuriy B. Trach, Lidia V. Bulgakova,
Oksana I. Makota, Wladimir Ya. Suprun,
Bärbel Schulze, Christian B.W. Stark**

Journal of Molecular Catalysis A: Chemical 302 (2009) 124

Vanadium diboride catalyzed oxidation of cyclooctene by molecular oxygen: Kinetic study

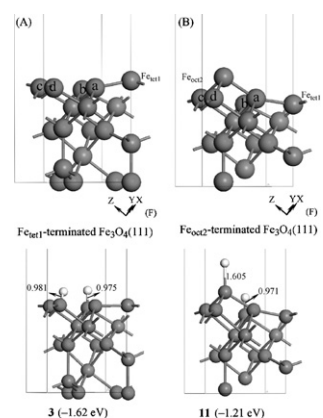
The kinetics of initial stages of the liquid-phase oxidation of cyclooctene by molecular oxygen catalyzed by VB_2 has been reported for the first time. The reaction rate was depended on cyclooctene concentration with less than first order. The kinetic model of oxidation process has been proposed. The equation for the reaction rate which quantitatively describe the obtained experimental dependences has been evaluated from this model.



**Tao Yang, Xiao-Dong Wen, Chun-Fang Huo,
Yong-Wang Li, Jianguo Wang, Haijun Jiao**

Journal of Molecular Catalysis A: Chemical 302 (2009) 129

Structure and energetics of hydrogen adsorption on $\text{Fe}_3\text{O}_4(111)$

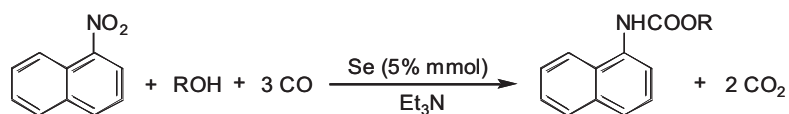


Xiaopeng Zhang, Huanzhi Jing

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A facile one-pot phosgene-free synthesis of naphthalen-1-ylcarbamates by selenium-catalyzed carbonylation of 1-nitronaphthalene with carbon monoxide

With selenium as catalyst and triethylamine as cocatalyst, the facile one-pot selenium-catalyzed redox carbonylation of 1-nitronaphthalene with a series of alcohols and carbon monoxide proceeds efficiently to afford the corresponding naphthalen-1-ylcarbamates in fair to good yields.



**Pravin R. Likhari, R. Arundhathi, Sutapa Ghosh,
M. Lakshmi Kantam**

Journal of Molecular Catalysis A: Chemical 302 (2009) 142

Polyaniline nanofiber supported FeCl_3 : An efficient and reusable heterogeneous catalyst for the acylation of alcohols and amines with acetic acid

An efficient and reusable polyaniline nanofiber supported ferric chloride catalyst was developed and characterized by FT-IR, UV-vis, XPS, TEM and XRD techniques. The catalyst was used in the selective acylation of alcohols and amines employing acetic acids as acylating agents to obtain the corresponding acetate and acetamide in good to excellent yield.

