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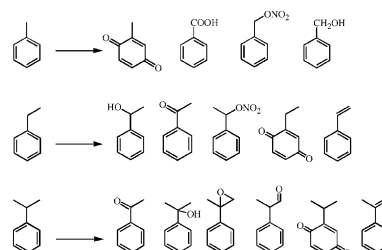
Articles

**Susana L.H. Rebelo, Mário M.Q. Simões,
M. Graça P.M.S. Neves,
José A.S. Cavaleiro**

Journal of Molecular Catalysis A: Chemical
201 (2003) 9

Oxidation of alkylaromatics with hydrogen peroxide catalysed by manganese (III) porphyrins in the presence of ammonium acetate

The oxidation of toluene, ethylbenzene and cumene with H_2O_2 , in the presence of several manganese(III) porphyrins with electron-withdrawing substituents, was studied using ammonium acetate as a co-catalyst. All products were characterised and their formation was justified by studying the oxidation of primary precursors. The formation of the nitrate compounds was shown to be dependent on the presence of ammonium acetate.

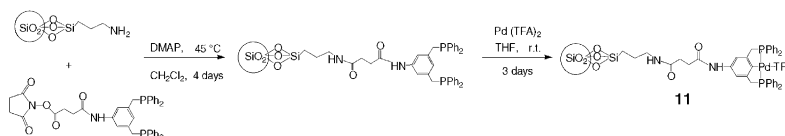


Ratana Chanthateyanonth, Howard Alper

Journal of Molecular Catalysis A: Chemical
201 (2003) 23

The first synthesis of stable palladium(II) PCP-type catalysts supported on silica—application to the Heck reaction

An efficient method for the formation of a silica-immobilized tridentate diphosphinoaryl ligand (PCP-type) palladium(II) complex (**11**) is described and successfully used as a catalyst for the Heck reaction.

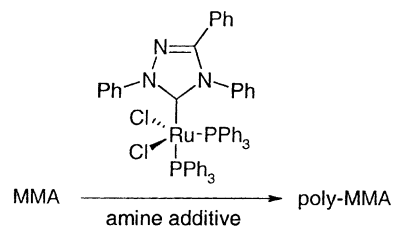


Karen Melis, Francis Verpoort

Journal of Molecular Catalysis A: Chemical
201 (2003) 33

$RuCl_2(PPh_3)_2$ (triazol-5-ylidene): an active catalyst for controlled radical polymerization of methyl methacrylate in the presence of primary or secondary amines

Addition of primary and secondary amine to the $RuCl_2(PPh_3)_2$ (triazol-5-ylidene)/ethyl-2-bromo-isobutyrate initiating system provides a highly active catalyst for the controlled radical polymerization of methyl methacrylate. Polymers with a very narrow molecular weight distribution (MWD=1.24) are obtained within 24 h of reaction.

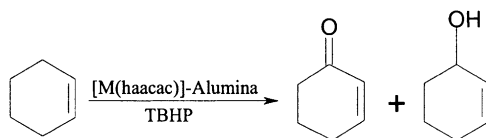


M. Salavati-Niasari, S.H. Banitaba

Journal of Molecular Catalysis A: Chemical
201 (2003) 43

Alumina-supported Mn(II), Co(II), Ni(II) and Cu(II) bis(2-hydroxyanil)acetylacetonate complexes as catalysts for the oxidation of cyclohexene with *tert*-butylhydroperoxide

New Mn(II), Co(II), Ni(II) and Cu(II) complexes of a tetradentate Schiff base ligand [bis(2-hydroxyanil)acetylacetonate], "2-[(1-methyl-3-[(2-hydroxyphenyl)imino]butylidene)-amino]phenol", H₂haacac, have been prepared and characterized by elemental analysis, IR spectroscopy and conductometric method. Alumina-supported [M(haacac)] complexes catalyze the oxidation of cyclohexene with *tert*-butylhydroperoxide (TBHP). The major products of the reaction were 2-cyclohexene-1-ol (OH), 2-cyclohexene-1-one (C=O). The effect of temperature, solvent and time on the oxidation reaction have been studied. Mn(haacac)-alumina shows significantly higher catalytic activity than other alumina-supported complexes.

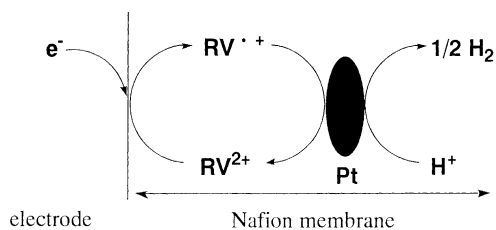


**Toshiyuki Abe, Takaki Fujita,
Kouki Sekimoto, Akio Tajiri,
Masao Kaneko**

Journal of Molecular Catalysis A: Chemical
201 (2003) 55

Electrochemical hydrogen evolution by catalyst membrane composed of platinum, alkyl viologen and Nafion: consideration of the kinetically dominant factor based on understanding of electron-mediating ability of the viologen molecule

Electrocatalytic H₂ formation was carried out by using a Nafion membrane embedding a Pt catalyst as well as an alkyl viologen (RV²⁺), in which the H⁺ reduction catalyzed by Pt via electrogenerated RV^{•+} was examined in terms of kinetics. The dominant factor that affects the overall kinetics in the present catalysis system was discussed.

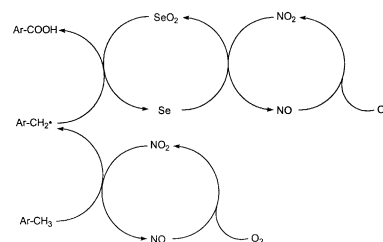


Joseph E. Remias, Ayusman Sen

Journal of Molecular Catalysis A: Chemical
201 (2003) 63

Nitrogen oxides/selenium dioxide-mediated benzylic oxidations

The oxidation of benzylic groups to the corresponding carboxylic acid functionality by dioxygen has been found to be mediated by a combination of nitric oxide (NO) and selenium dioxide (SeO₂). Substrates examined include alkylnaphthalenes and alkyipyridines. The aldehyde appears to be an intermediate in the reaction. Mechanistic studies suggest that the rate-determining step is hydrogen atom abstraction by nitrogen dioxide (NO₂) to form the benzyl radical. Selenium dioxide subsequently oxidizes this radical to the desired product.

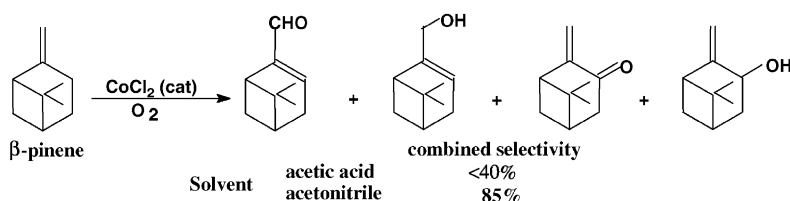


**Márcio J. da Silva,
Patricia Robles-Dutenhefner,
Luciano Menini, Elena V. Gusevskaya**

Journal of Molecular Catalysis A: Chemical
201 (2003) 71

Cobalt catalyzed autoxidation of monoterpenes in acetic acid and acetonitrile solutions

A novel selective CoCl₂ catalyzed oxidation of β-pinene in acetonitrile solutions resulting in allylic oxygenated derivatives has been developed. In acetic acid, the reaction is complicated by the substrate isomerization and acetic acid addition. Limonene and α-pinene give both allylic oxidation and epoxidation products (molar ratio ≈ 1/1), with chemoselectivities being higher in acetonitrile than those in acetic acid.

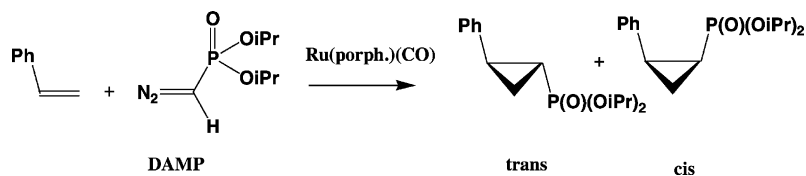


**Christine Paul-Roth,
Frédéric De Montigny,
Gildas Rethoré, Gérard Simonneaux,
Mihaela Gulea, Serge Masson**

Journal of Molecular Catalysis A: Chemical
201 (2003) 79

Cyclopropanation of alkenes with diisopropyl diazomethylphosphonate catalysed by ruthenium porphyrin complexes

Stereoselectivities, regioselectivities and yields for cyclopropanation reactions of diisopropyl diazomethylphosphonate with styrene derivatives, catalysed by ruthenium porphyrins, are reported.

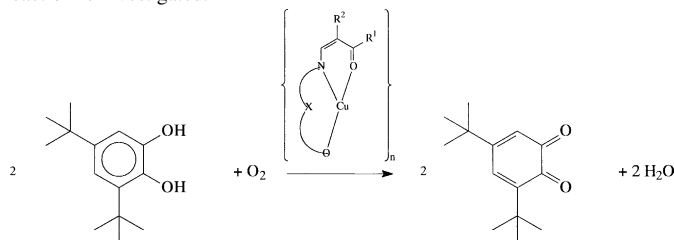


**Rainer Wegner, Michael Gottschaldt,
Wolfgang Poppitz, Ernst-G. Jäger,
Dieter Klemm**

Journal of Molecular Catalysis A: Chemical
201 (2003) 93

Catechol oxidase model compounds based on aminocarbohydrates: new structure types and investigations on the catalytic reaction

Copper(II) complexes with β -ketoenaminic ligands based on aminocarbohydrates are efficient model compounds for catechol oxidase. The present work contains new compounds of this series. The influence of competitive inhibitors, the pH-value and of simple ligands like chloride on the reaction is investigated.

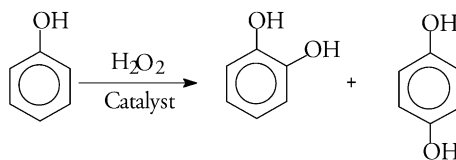


**Mannar R. Maurya, Salam J.J. Titinchi,
Shri Chand**

Journal of Molecular Catalysis A: Chemical
201 (2003) 119

Oxidation of phenol with H_2O_2 catalysed by Cu(II), Ni(II) and Zn(II) complexes of N,N' -bis-(salicylidene)diethylenetriamine (H_2 saldien) encapsulated in Y-zeolite

Encapsulation of Cu(II), Ni(II) and Zn(II) complexes of N,N' -bis-(salicylidene) diethylenetriamine (H_2 saldien) in zeolite-Y and their catalytic activity towards the decomposition of H_2O_2 and oxidation of phenol are reported.

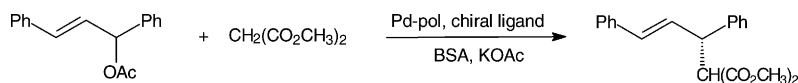


**Maria Michela Dell'Anna,
Piero Mastrorilli,
Cosimo Francesco Nobile,
Gian Paolo Suranna**

Journal of Molecular Catalysis A: Chemical
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Asymmetric allylic alkylation using a polymer-supported palladium catalyst in the presence of chiral ligands

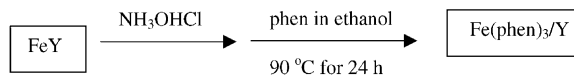
Polymer-supported $Pd(AAEMA)_2$ [$AAEMA^-$: deprotonated form of 2-(acetoacetoxy)ethyl methacrylate] in the presence of chiral ligands catalyses the asymmetric substitution of *rac*-1,3-diphenyl-2-propenyl acetate with dimethyl malonate.



Binbin Fan, Weibin Fan, Ruifeng Li

Journal of Molecular Catalysis A: Chemical
201 (2003) 137

Fe-containing Y as a host for the preparation
of a ship-in-a-bottle catalyst

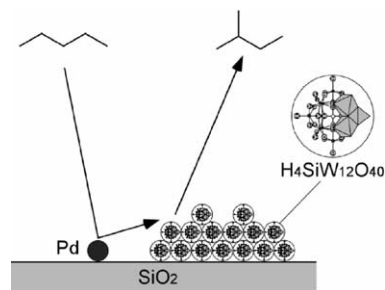


**Atsuyuki Miyaji, Tsuneo Echizen,
Kohichi Nagata, Yusuke Yoshinaga,
Toshio Okuhara**

Journal of Molecular Catalysis A: Chemical
201 (2003) 145

Selective hydroisomerization of *n*-pentane
to isopentane over highly dispersed Pd-
H₄SiW₁₂O₄₀/SiO₂

The catalyst with the composition of
1 wt.%Pd-20 wt.% H₄SiW₁₂O₄₀/SiO₂ was
highly active and selective for *n*-pentane
isomerization. The dispersion of
H₄SiW₁₂O₄₀ on SiO₂ was estimated to be
about 0.4 from the adsorption of benzonitrile,
and the acid strength was suppressed on SiO₂.

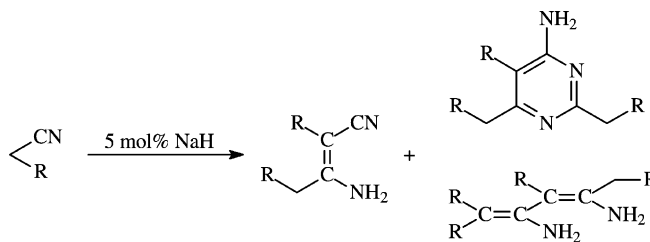


**Xiaochun Tao, Taoping Liu, Hui Tao,
Ruzhang Liu, Yanlong Qian**

Journal of Molecular Catalysis A: Chemical
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Selective oligomerization of nitriles having
 α -hydrogen catalyzed by alkali

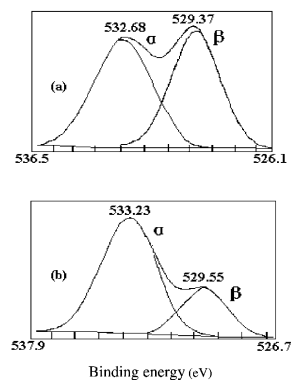
Highly selective cyclotrimerization of acetonitrile was achieved in the presence of a catalytic amount of sodium hydride under mild conditions to produce 4-amino-2,6-dimethylpyrimidine in satisfactory yields. This catalytic system is also efficient for reactions of other nitriles having α -hydrogen. Linear dimers, linear- or cyclo-trimers can be obtained selectively.

**MinChen, Xiao-Ming Zheng**

Journal of Molecular Catalysis A: Chemical
201 (2003) 161

Effect of promoter thallium for a novel selectivity
oxidation catalyst studied by X-ray
photoelectron spectroscopy

XPS was used to study the novel series of V-
Cs-Cu-Tl catalyst, which was used for the
selective oxidation reaction to produce *p*-*tert*-
butyl benzaldehyde. The optimum catalytic
activity ascribed to the promoter thallium can
effectively enhanced the redox cycle of
V⁵⁺ ↔ V⁴⁺. The O 1s analysis of catalyst
indicated that the nucleophilic oxygen (O²⁻)
on the catalyst surface plays an important role
in this selectivity oxidation.

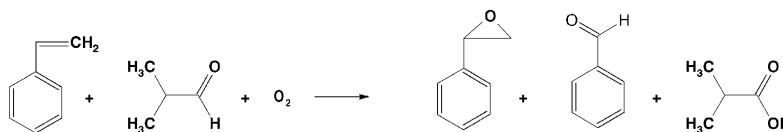


J. Haber, M. Kłosowski, J. Pottowicz

Journal of Molecular Catalysis A: Chemical
201 (2003) 167

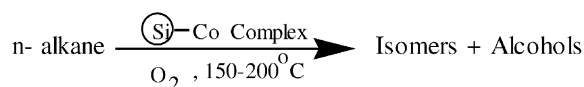
Co-oxidation of styrene and *iso*-butyraldehyde in the presence of polyaniline-supported metalloporphyrins

Co-oxidation of styrene and *iso*-butyraldehyde with gas phase oxygen in the temperature range 20–35 °C has been studied in the presence of Co-, Fe- and Mn-T(*p*-SO₃H)PP porphyrins in the liquid phase and supported on polyaniline (PANI) as catalysts. Supporting the porphyrin molecules on polyaniline modifies their catalytic properties. The mechanisms of the two parallel reaction pathways to benzaldehyde and epoxystyrene are discussed.

**Amit Kumar, Gopal S. Mishra, Anil Kumar**

Journal of Molecular Catalysis A: Chemical
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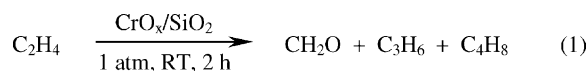
Covalently bonded Schiff base cobalt complex catalyst for the selective oxidation of linear alkanes using molecular oxygen

**Boping Liu, Hisayuki Nakatani, Minoru Terano**

Journal of Molecular Catalysis A: Chemical
201 (2003) 189

Mechanistic implications of the unprecedented transformations of ethene into propene and butene over Phillips CrO_x/SiO₂ catalyst during induction period

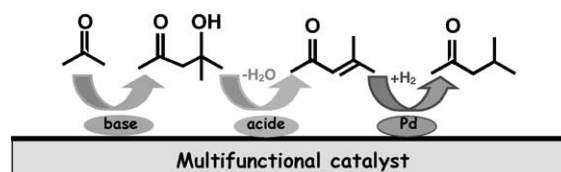
An industrial calcined Phillips CrO_x/SiO₂ catalyst engaged in induction period under inter-action with ethene at ambient conditions was studied by temperature-programmed desorption (TPD). We got the unprecedented evidence that the first hydrocarbon species, that is propene formed after the generation of formaldehyde, had already been produced on the catalyst followed by the formation of the second hydrocarbon species butene (shown in Eq. (1)) during the induction period implying an ethene metathesis initiation.

**María de Jesús Martínez-Ortiz, Didier Tichit, Philippe Gonzalez, Bernard Coq**

Journal of Molecular Catalysis A: Chemical
201 (2003) 199

The “one-pot” synthesis of 4-methyl-2-pentanone (methyl isobutyl ketone) from acetone over PdCu catalysts prepared from layered double hydroxides

Reaction scheme for the “one-pot” synthesis of MIBK from acetone over multifunctional catalysts prepared from LDH precursors.

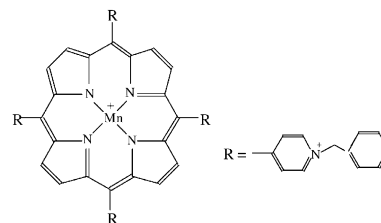


**F.C. Skrobot, A.A. Valente,
G. Neves, I. Rosa, J. Rocha
J.A.S. Cavaleiro**

Journal of Molecular Catalysis A: Chemical
201 (2003) 211

Monoterpenes oxidation in the presence of Y zeolite-entrapped manganese(III) tetra(4-N-benzylpyridyl)porphyrin

Manganese(III) tetra(4-N-benzylpyridyl)porphyrin complex (MnTBzPyP) is active in the oxidation of monoterpenes at room temperature and atmospheric pressure. A detailed study on the characterization and catalytic performance of MnTBzPyP–NaY suggests the successful nano-inclusion of MnTBzPyP. This catalyst is more stable than its homogeneous counterpart, but leaching of the complex occurs.

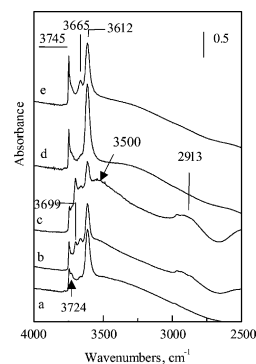


S. Todorova, B.-L. Su

Journal of Molecular Catalysis A: Chemical
201 (2003) 223

Propane as alkylating agent for benzene alkylation on bimetal Ga and Pt modified H-ZSM-5 catalysts: FTIR study of effect of pre-treatment conditions and the benzene adsorption

FTIR spectroscopy was used to study the influence of pre-treatment on OH groups of H-ZSM-5, Ga-ZSM-5, Pt-ZSM-5 and GaPt-ZSM-5 catalysts and the confinement of benzene molecules in these catalysts pretreated under different conditions. Types of the hydroxyl groups in GaPt-ZSM-5 and Ga-ZSM-5 are very sensitive to the pre-treatment. Benzene molecules can interact with different OH groups and form clusters in the zeolite channels. The location of benzene on Pt particles is discussed.



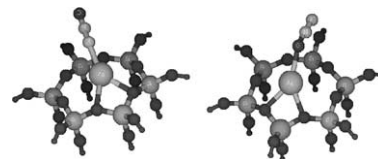
**N.U. Zhanpeisov, G. Martra, W.S. Ju,
M. Matsuoka, S. Coluccia, M. Anpo**

Journal of Molecular Catalysis A: Chemical
201 (2003) 237

Interaction of N₂O with Ag⁺ ion-exchanged zeolites: an FT-IR spectroscopy and quantum chemical ab initio and DFT studies

FT-IR spectroscopy and theoretical ab initio as well as density functional (DFT) methods have been applied to the investigation of the interaction of N₂O with Ag⁺ counter-cations in a ZSM-5 zeolite. It was observed that N₂O interacts with Ag⁺ centers in both the N-end and O-end down forms producing a superposition of peculiar ν₃ and ν₁ IR bands. According to DFT calculations, main ν₃ and weaker ν₁ modes of the N-end down form can be clearly observed in the experimental spectra, centered at 2256 and 1325 cm⁻¹ (high N₂O coverage), respec-

tively. As for IR absorptions due to the O-end down interaction of N₂O molecules with Ag⁺ ions, the ν₁ band, predicted by calculations, fall in the 1280–1250 cm⁻¹ ranges. However, it was not observable, because located below the low frequency limit of the IR transparency of the zeolite.

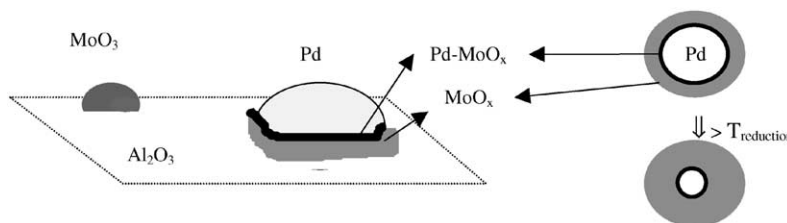


**A.M. Eberhardt, E.V. Benvenuti,
C.C. Moro, G.M. Tonetto, D.E. Damiani**

Journal of Molecular Catalysis A: Chemical
201 (2003) 247

NO decomposition on PdMo/γ-Al₂O₃ catalysts

NO decomposition reaction was studied on PdMo/γ-Al₂O₃ catalysts. The catalytic tests revealed that Pd-Mo catalysts show an increase of oxygen evolution at elevated temperatures and a longer steady state activity than Pd/γ-Al₂O₃ catalyst. Characterization studies suggest a decoration effect of Mo over Pd particle. This interaction appears to be responsible for the observed modification in NO activity and selectivity.

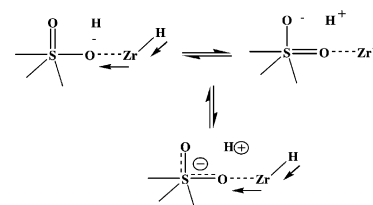


E. García, M.A. Volpe, M.L. Ferreira, E. Rueda

Journal of Molecular Catalysis A: Chemical 201 (2003) 263

A discussion of a mechanism for isomerization of *n*-butane on sulfated zirconia

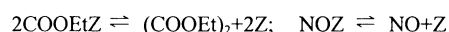
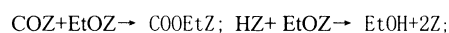
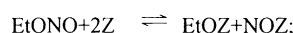
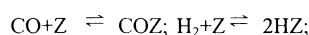
This scheme shows the proposed active superacidic Bronsted site on SZ in presence of *n*-butane. This site is the key of the mechanism presented in this manuscript. The hydride transfer to a Lewis Acidic Zr next to the Bronsted site is the first step of this active formation. Superacidity would arise because of the stabilization of the SO₂ moiety.



Fandong Meng, Genhui Xu, Qunrong Guo

Journal of Molecular Catalysis A: Chemical 201 (2003) 283

Kinetics of the catalytic coupling reaction of carbon monoxide to diethyl oxalate over Pd/α-Al₂O₃ catalyst

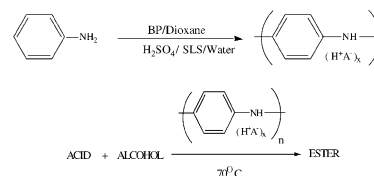


Malladi Sai Ram, Srinivasan Palaniappan

Journal of Molecular Catalysis A: Chemical 201 (2003) 289

Benzoyl peroxide oxidation route to polyaniline salt and its use as catalyst in the esterification reaction

Aniline was oxidized to polyaniline salt using benzoyl peroxide as an oxidizing agent in the presence of sulfuric acid and sodium lauryl sulfate surfactant. The polymer sample was characterized using infrared, X-ray diffraction, particle size, resistance and density measurements. Polyaniline salt was used as catalyst for the esterification reaction of carboxylic acids with methanol. The process is being reported for the first time. Preparation of catalyst, recovery and reusability of the catalyst are found to be good.



B.B. Marvey, J.A.K. du Plessis, H.C.M. Vosloo J.C. Mol

Journal of Molecular Catalysis A: Chemical 201 (2003) 297

Metathesis of unsaturated fatty acid esters derived from South African sunflower oil in the presence of a 3 wt.% Re₂O₇/SiO₂-Al₂O₃/SnBu₄ catalyst

The metathesis of methyl linoleate, oleate/linoleate methyl esters and a mixture of fatty acid esters derived from South African sunflower oil was investigated using the heterogeneous 3 wt% Re₂O₇/SiO₂-Al₂O₃/SnBu₄ catalyst system. Total conversions above 70% and total diester yields of ca. 20% were obtained. The catalyst system reached maximum catalytic activity at 60°C.

