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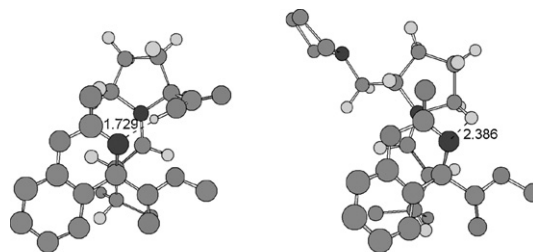
Articles

Hongliang Li, Aiping Fu, Haining Shi

Journal of Molecular Catalysis A: Chemical 303 (2009) 1

Theoretical studies of stereoselectivities in the direct organocatalytic Mannich reactions involving ketimine

The effects of two kinds of chiral secondary amine catalysts on the diastereoselectivities of the direct Mannich reactions between ketimine and aldehyde have been studied theoretically. The most stable transition states of the crucial C–C bond-forming step for the proline and (*S*)-1-(2-pyrrolidinylmethyl) pyrrolidine-catalyzed processes provide a good explanation for the opposite diastereoselectivities of these two different kinds of catalysts.



anti-re-si-proline

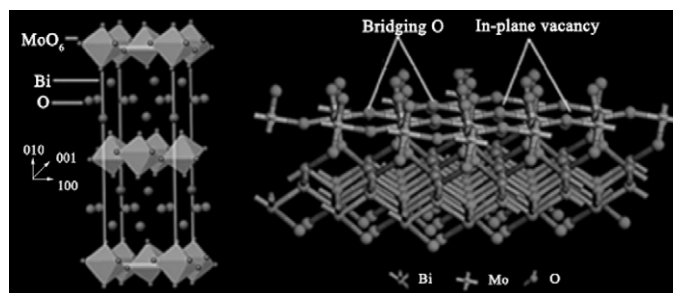
anti-si-si-(S)-1-(2-pyrrolidinylmethyl) pyrrolidine

Yan Zheng, Fang Duan, Ju Wu, Liang Liu, Mingqing Chen, Yi Xie

Journal of Molecular Catalysis A: Chemical 303 (2009) 9

Enhanced photocatalytic activity of bismuth molybdates with the preferentially exposed {0 1 0} surface under visible light irradiation

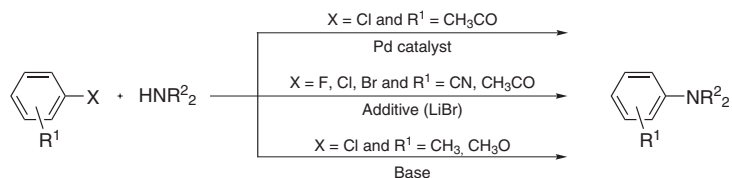
From the structure of the stoichiometric bismuth molybdates (0 1 0) surface, the larger sheets sample with the preferentially exposed {0 1 0} surface of the largely distorted Mo–O octahedra supply more oxygen defects and in-plane vacancies, which enhances the concentration of ·OH and/or ·OOH radicals and thus greatly improves the photocatalytic property of γ -Bi₂MoO₆.



Wolfgang Kleist, Sandra S. Pröckl, Markus Drees, Klaus Köhler, Laurent Djakovitch

Journal of Molecular Catalysis A: Chemical 303 (2009) 15

Amination of aryl chlorides and fluorides toward the synthesis of aromatic amines by palladium-catalyzed route or transition metal free way: Scopes and limitations

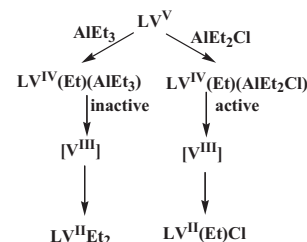


Igor E. Soshnikov, Nina V. Semikolenova, Konstantin P. Bryliakov, Vladimir A. Zakharov, Carl Redshaw, Evgenii P. Talsi

Journal of Molecular Catalysis A: Chemical 303 (2009) 23

An EPR study of the vanadium species formed upon interaction of vanadyl N and C-capped tris(phenolate) complexes with AlEt_3 and AlEt_2Cl

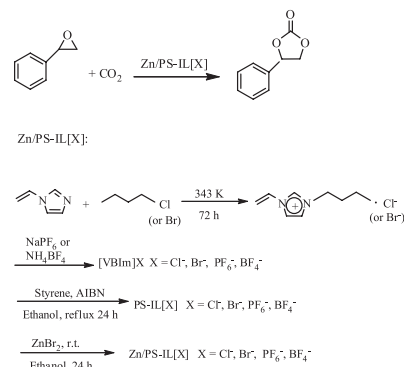
The vanadium(V) complexes of N and C-capped tripodal ligands (complexes **1** and **2**, respectively) serve as active, thermally robust pro-catalysts for ethylene homo- and ethylene/propylene copolymerization. EPR spectroscopic studies of the systems **1(2)**/ AlEt_2Cl , and **1(2)**/ $\text{AlEt}_2\text{Cl}/\text{ETA}$ (ETA = trichloroacetate) show, that the concentration of V(IV) species in the reaction solution correlates with the polymerization activity of the **1(2)**/ AlEt_2Cl catalyst systems and complexes of the type $\text{LV}^{\text{IV}}(\text{Et})(\text{AlEt}_2\text{Cl})$ can be precursors of the active species of polymerization of the catalyst systems **1(2)**/ AlEt_2Cl .



Kun Qiao, Fumitaka Ono, Quanxi Bao, Daisuke Tomida, Chiaki Yokoyama

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Efficient synthesis of styrene carbonate from CO_2 and styrene oxide using zinc catalysts immobilized on soluble imidazolium–styrene copolymers

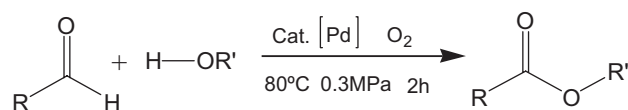


Yanyan Diao, Ruiyi Yan, Suojiang Zhang, Pu Yang, Zengxi Li, Lei Wang, Haifeng Dong

Journal of Molecular Catalysis A: Chemical 303 (2009) 35

Effects of Pb and Mg doping in Al_2O_3 -supported Pd catalyst on direct oxidative esterification of aldehydes with alcohols to esters

The Pb, Mg-doped Al_2O_3 -supported Pd crystals were prepared, characterized and used as catalysts for the oxidative esterification of aldehydes with alcohols and oxygen to corresponding esters. The catalytic activities of the doped and undoped Pd catalysts were examined in the presence and absence of oxygen to evaluate the effects of Pb and Mg.

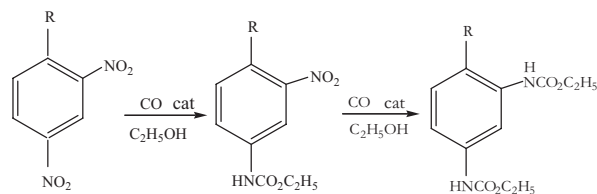


Monika Karpińska, Jadwiga Skupińska, Piotr Baran

Journal of Molecular Catalysis A: Chemical 303 (2009) 43

Carbonylation of aromatic dinitro compounds with carbon monoxide to respective dicarbamates in the presence of the $\text{PdCl}_2/\text{Fe}/\text{I}_2/\text{Py}$ catalytic system

The object of the study was the reductive carbonylation of 1,3-dinitrobenzene, 1,4-dinitrobenzene and 2,4-dinitrotoluene to respective dicarbamates in the presence of $\text{PdCl}_2/\text{Fe}/\text{I}_2/\text{Py}$ catalytic system. By raising the catalyst amount and by extending the carbonylation reaction time a 100% conversion of dinitrobenzene to corresponding dicarbamates was achieved, with a selectivity of 87, 68, and 55% for 1,4-, 1,3-dinitrobenzene and 2,4-dinitrotoluene, respectively.



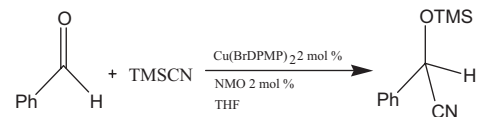
Cat: $\text{PdCl}_2/\text{Fe}/\text{I}_2/\text{Py}$, R = CH_3 , H (1,3 and 1,4 dinitro).

**K. Kanmani Raja, D. Easwaramoorthy,
S. Kutti Rani, J. Rajesh, Y. Jorapur,
S. Thambidurai, PR. Athappan,
G. Rajagopal**

Journal of Molecular Catalysis A: Chemical 303 (2009) 52

Synthesis, spectral, electrochemical and catalytic properties of Cu(II), Ni(II) and Co(II) complexes containing N, O donors

Metal(II) chelates of Schiff bases derived from the condensation of multi-substituted aniline with mono- and di-substituted salicylaldehyde have been prepared and characterized by ¹H NMR, IR, electronic, ESR, magnetic and cyclic voltammetry measurements. Cu(Br-DPMP)₂ was found to be an efficient catalyst for cyanosilylation of aldehydes under mild conditions.

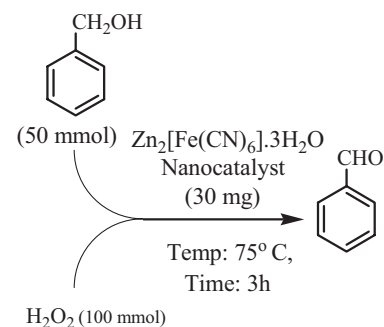


**S.R. Ali, V.K. Bansal, A.A. Khan, S.K. Jain,
M.A. Ansari**

Journal of Molecular Catalysis A: Chemical 303 (2009) 60

Growth of zinc hexacyanoferrate nanocubes and their potential as heterogeneous catalyst for solvent-free oxidation of benzyl alcohol

Zinc hexacyanoferrate nanocubes with size ranging from 63 to 164 nm have been synthesized and characterized. Catalytic activity of nanocubic zinc hexacyanoferrate has been studied for solvent-free oxidation of benzyl alcohol to benzaldehyde using H₂O₂ as oxidant.

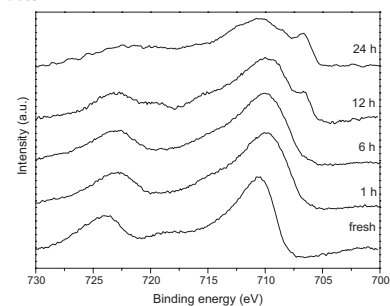


**Mingyue Ding, Yong Yang, Baoshan Wu, Jian Xu,
Chenghua Zhang, Hongwei Xiang, Yongwang Li**

Journal of Molecular Catalysis A: Chemical 303 (2009) 65

Study of phase transformation and catalytic performance on precipitated iron-based catalyst for Fischer–Tropsch synthesis

Detailed phase transformation in syngas (H₂/CO = 1.2) and Fischer–Tropsch synthesis performances of a precipitated iron-based catalyst were studied in a slurry-phase continuously stirred tank reactor. The hematite reduced firstly to magnetite with increasing reduction time, and then the bulk Fe₃O₄ reached gradually a steady state, accompanied with the slow conversion of the surface magnetite to iron carbides.

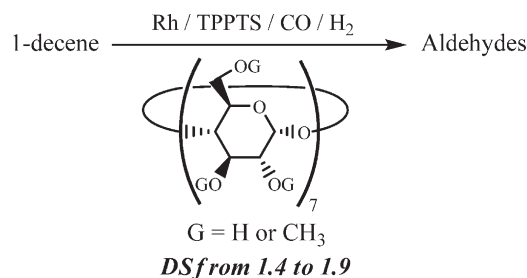


**François-Xavier Legrand, Mathieu Sauthier,
Christophe Flahaut, Johan Hachani, Claire Elfakir,
Sophie Fourmentin, Sébastien Tilloy,
Eric Monflier**

Journal of Molecular Catalysis A: Chemical 303 (2009) 72

Aqueous hydroformylation reaction mediated by randomly methylated β-cyclodextrin: How substitution degree influences catalytic activity and selectivity

A crude mixture of randomly methylated β-cyclodextrin (RAME-β-CD) has been fractionated to evaluate the influence of the methylation degree on activity and selectivity of a rhodium/TPPTS catalytic system in hydroformylation of 1-decene. The catalytic activity was found to gradually increase with the number of methyl groups on the CD whereas the chemoselectivity and regioselectivity remained unchanged.

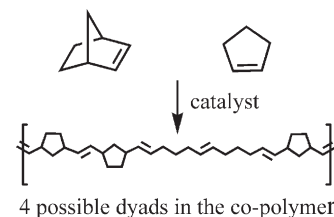


**Margaret M. Gallagher, A. Denise Rooney,
John J. Rooney**

Journal of Molecular Catalysis A: Chemical 303 (2009) 78

Metathesis co-polymerization as a means of comparing the reactivity of ruthenium initiators in conventional solvents and ionic liquids

Ring opened metathesis polymerization was carried out on a number of cyclic olefins using $\text{Cl}_2(\text{PCy}_3)_2\text{Ru}[\text{CH}(\text{Ph})]$ and $[(\eta^6\text{-}p\text{-cymene})(\text{PCy}_3)\text{RuCl}(\text{=C=C=CPh}_2)] \text{OTf}$ in dichloromethane and a range of ionic liquids. Microstructural parameters were determined from the ^{13}C NMR spectra recorded of the polymers. The findings indicate that an increase in activity of both catalysts can occur in certain ionic liquids systems.

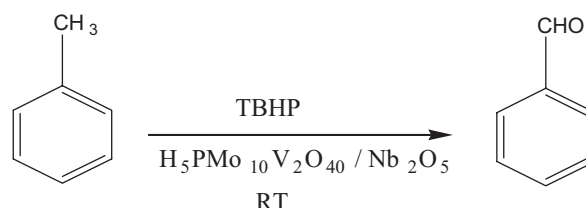


**K.T. Venkateswara Rao, P.S.N. Rao, P. Nagaraju,
P.S. Sai Prasad, N. Lingaiah**

Journal of Molecular Catalysis A: Chemical 303 (2009) 84

Room temperature selective oxidation of toluene over vanadium substituted polyoxometalate catalysts

Selective oxidation of toluene to benzaldehyde is achieved at room temperature over heterogeneous niobia supported vanadium incorporated molybdophosphoric acid catalyst. The present catalyst is highly active, selective towards benzaldehyde and reusable with out any appreciable loss in activity and selectivity.

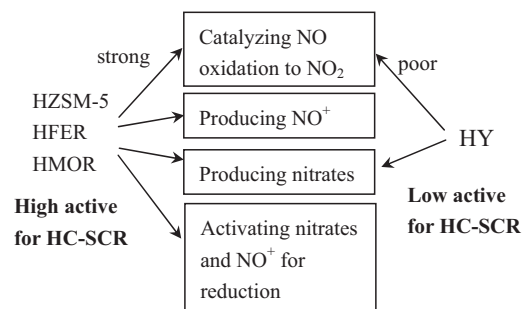


**Xiaofei Ma, Xiping Wang, Ran Bi, Zhen Zhao,
Hong He**

Journal of Molecular Catalysis A: Chemical 303 (2009) 90

Defect of HY as catalyst for selective catalytic reduction of NO in comparison with the pentasil zeolites

Specific behavior of HY in some processes that are possible reaction steps of the selective catalytic reduction of NO by hydrocarbon (HC-SCR) was investigated comparing to those of the pentasil zeolites. It indicated that the following functions of HY weaker than those of the pentasil zeolites should be strengthen for designing practical HC-SCR catalysts based on the zeolite.

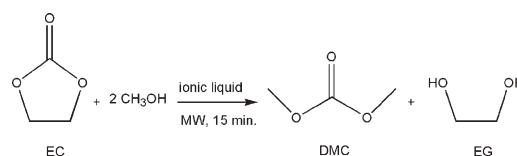


**Manju Mamparabath Dharman, Hye-Young Ju,
Hye-Lim Shim, Mi-Kyung Lee, Kyung-Hoon Kim,
Dae-Won Park**

Journal of Molecular Catalysis A: Chemical 303 (2009) 96

Significant influence of microwave dielectric heating on ionic liquid catalyzed transesterification of ethylene carbonate with methanol

The efficiency of microwave heating over conventional transesterification reaction and the heating characteristics of transesterification reaction mixture in the presence of ionic liquids were investigated. The microwave specific heating provided a rapid and sustainable approach for transesterification of ethylene carbonate with methanol.

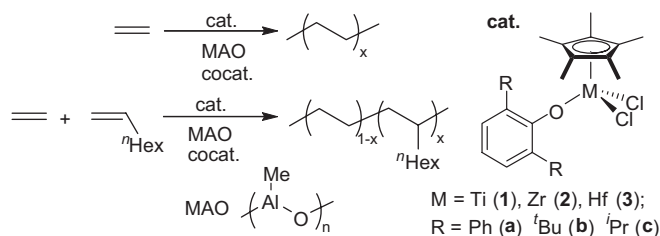


Koji Itagaki, Shinya Hasumi, Michiya Fujiki, Kotohiro Nomura

Journal of Molecular Catalysis A: Chemical 303 (2009) 102

Ethylene polymerization and ethylene/1-octene copolymerization using group 4 half-metallocenes containing aryloxo ligands, Cp* $MCl_2(OAr)$ [$M = Ti, Zr, Hf$; Ar = O-2,6- $R_2C_6H_3$, R = ^tBu, Ph]—MAO catalyst systems

Effect of the centered metal in ethylene (co)polymerization using a series of Cp* $MCl_2(O-2,6-R_2C_6H_3)$ in the presence of MAO cocatalyst have been explored; the catalytic activities as well as comonomer (1-octene) incorporations were highly affected by the centered metal employed rather than the phenoxy substituents.

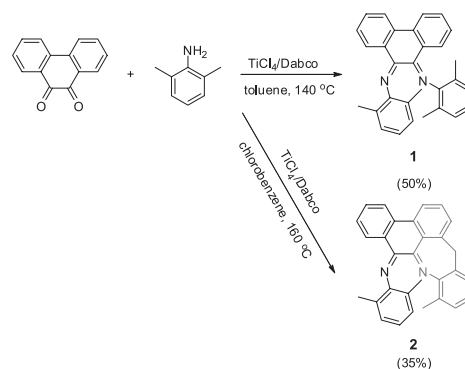


Lidong Li, Manseong Jeon, Sang Youl Kim

Journal of Molecular Catalysis A: Chemical 303 (2009) 110

Synthesis, characterization and ethylene polymerisation of 9,10-phenanthrenequinone-based nickel(II)- α -diimine complexes

Two 9,10-phenanthrenequinone-based α -diimine ligands **1** and **2** were prepared by condensation of 2,6-dimethylaniline and 9,10-phenanthrenequinone in the presence of the $TiCl_4/1,4$ -diazabicyclo[2.2.2]octane catalytic system in a one-pot reaction. Reaction of ligands **1** and **2** with $(DME)NiBr_2$ in dichloromethane at room temperature led to nickel complexes **3** and **4**, respectively, which can polymerise ethylene with good activities in the presence of MAO as activator.

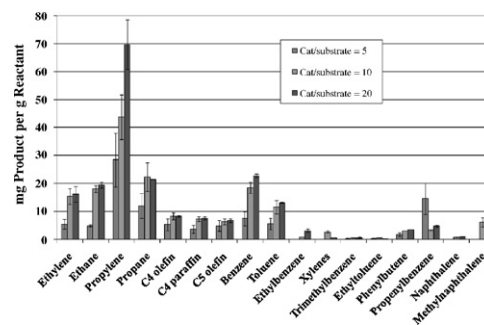


Tracy J. Benson, Rafael Hernandez, W. Todd French, Earl G. Alley, William E. Holmes

Journal of Molecular Catalysis A: Chemical 303 (2009) 117

Elucidation of the catalytic cracking pathway for unsaturated mono-, di-, and triacylglycerides on solid acid catalysts

Heterogeneous cracking reactions of unsaturated acylglyceride model compounds were investigated to determine the reaction pathway towards deoxygenation. Mono-, di-, and triolein were reacted at 400 °C over H⁺ZSM-5, faujasite, and silica–alumina catalysts. Reactions were carried out using a pulse-type microreactor utilizing online GC analysis. Results indicated the removal of the heteroatom by formation of CO and CO₂. These results reveal the potential of using lipid feedstocks for transportation fuels.

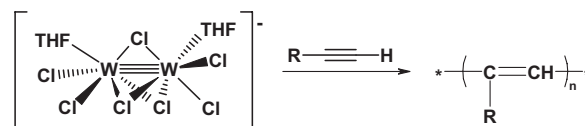


Nikolaos Saragas, Georgios Floros, Patrina Paraskevopoulou, Nikolaos Psaroudakis, Spyros Koinis, Marinos Pitsikalas, Konstantinos Mertis

Journal of Molecular Catalysis A: Chemical 303 (2009) 124

Polymerization of terminal alkynes with a triply bonded tungsten halo-complex

The triply bonded, triply halo-bridged complex $\text{Na}[\text{W}_2(\mu\text{-Cl})_3\text{Cl}_4(\text{THF})_2] \cdot (\text{THF})_3$ (W_2^{6+} , a^2e^4) is an efficient single-component initiator for the high-yield homogeneous or heterogeneous polymerization of monosubstituted alkynes. The bulk of the alkyl substituents does not significantly affect the yield of the reaction. The conditions dictate the microscopic structure of the polymers formed. The polymerization of phenylacetylene (**PA**) in THF is multimodal involving both polymerization and equilibration/depolymerization steps. Directly obtained evidence by ¹H NMR indicate the metathetical nature of the polymerization.

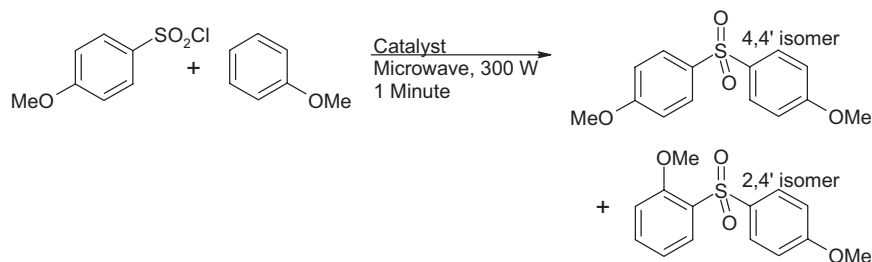


R = Ph, C₇H₇ (o-methylphenyl), C₇H₄F₃ (o-trifluoromethylphenyl), ⁿBu, ^tBu, Me₃Si, C₁₀H₇ (naphthyl)

Melissa Cooke, James Clark, Simon Breeden*Journal of Molecular Catalysis A: Chemical* 303 (2009) 132

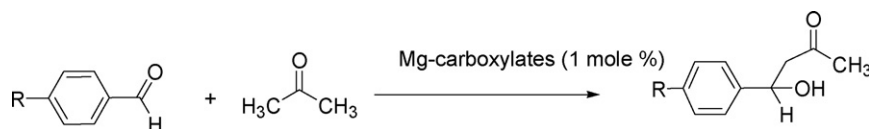
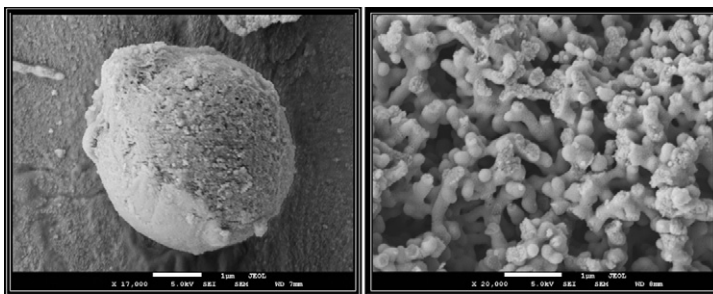
Lewis acid catalysed microwave-assisted synthesis of diaryl sulfones and comparison of associated carbon dioxide emissions

In this publication a range of diaryl sulfones were synthesised using a variety of hetero- and homogeneous Lewis acid catalysts in good yields under microwave activation. The carbon dioxide emissions associated with the reactions were estimated to compare environmental performance in the form of a new green chemistry metric.

**Bikash K. Dey, Anirban Karmakar, Jubaraj B. Baruah***Journal of Molecular Catalysis A: Chemical* 303 (2009) 137

Characterisation of magnesium carboxylates and their catalytic C–C bond formation reactions

Two magnesium (II) benzoate complexes are prepared by reacting magnesium with methanol in the presence of corresponding benzoic acids. These complexes are moderate catalysts for carbon–carbon bond formation between aromatic aldehydes and acetone. Characterization of these complexes and their role as catalysts for condensation reactions of acetone with different aldehydes are presented.

**Jian-wen Shi, Shao-hua Chen, Shu-mei Wang, Peng Wu, Gui-hua Xu***Journal of Molecular Catalysis A: Chemical* 303 (2009) 141Favorable recycling photocatalyst TiO₂/CFA: Effects of loading method on the structural property and photocatalytic activityIn order to more easily separate TiO₂ photocatalyst from the treated wastewater, TiO₂ was immobilized on the surface of coal fly ash (CFA) by employing a new and simple method, hybrid slurry procedure. The surface of TiO₂ layer covered on CFA is very rough. Furthermore, it is interesting that a three-dimensional network structure appears in the TiO₂-coated CFA.**Sébastien Leveneur, Dmitry Yu. Murzin, Tapio Salmi***Journal of Molecular Catalysis A: Chemical* 303 (2009) 148

Application of linear free-energy relationships to perhydrolysis of different carboxylic acids over homogeneous and heterogeneous catalysts

The goal of this work was to study the influence of the carbon chain length of the carboxylic acid on the perhydrolysis reaction using linear free-energy relations. A comparison between homogeneous and heterogeneous catalysis system was carried out, based on the apparent rate constant and on the analysis of the kinetic expression.

