



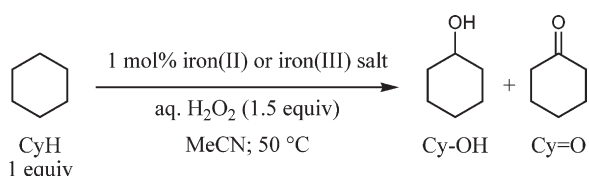
## Contents

### Articles

**Brandon Retcher, José Sánchez Costa, Jinkui Tang, Ronald Hage, Patrick Gamez, Jan Reedijk**

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Unexpected high oxidation of cyclohexane by Fe salts and dihydrogen peroxide in acetonitrile

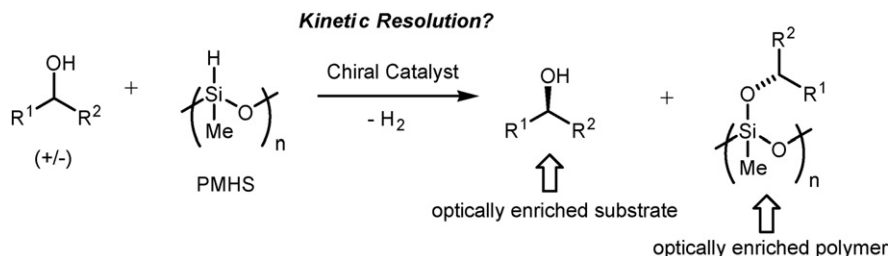


**Jean Thomas Issenhuth, Samuel Dagorne, Stéphane Bellemin-Laponnaz**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 6

A practical concept for the kinetic resolution of a chiral secondary alcohol based on a polymeric silane

Preliminary studies on the use of PMHS as a functionalizable polymer and hydride source for the kinetic resolution of secondary alcohols via Cu(I)-catalyzed dehydrogenative silylating process is reported and discussed.

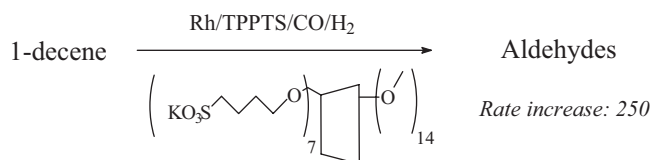


**D. Kirschner, M. Jaramillo, T. Green, F. Hapiot, L. Leclercq, H. Bricout, E. Monflier**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 11

Fine tuning of sulfoalkylated cyclodextrin structures to improve their mass-transfer properties in an aqueous biphasic hydroformylation reaction

A  $\beta$ -cyclodextrin sulfobutylated on its primary face and methylated on its secondary face was found to be the best cyclodextrin ever used as mass-transfer promoter in a biphasic rhodium-catalyzed hydroformylation reaction. The surface-active properties and the accessibility to the CD cavity appear to be the key parameters to explain the efficiency of this cyclodextrin.

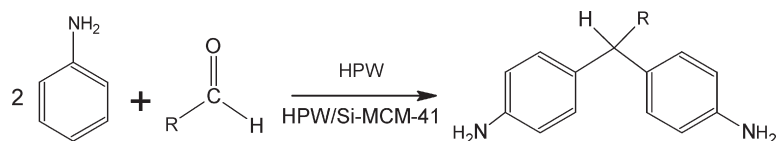


**S. Ajaikumar, A. Pandurangan**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 21

HPW and supported HPW catalyzed condensation of aromatic aldehydes with aniline: Synthesis of DATPM derivatives

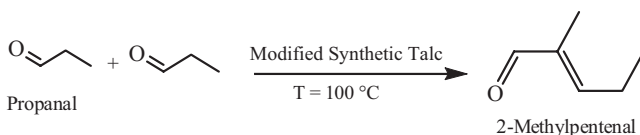
The Si-MCM-41 was synthesized by hydrothermal method and various wt.% (20 and 30 wt.%) of HPW were loaded on Si-MCM-41 by wet impregnation method. The synthesized catalysts were characterized by XRD, BET, FT-IR, TEM and TGA-DTG techniques. The catalytic activity of the catalyst was tested over the condensation reaction of aniline with various aromatic aldehydes.

**Hasmukh A. Patel, Sumeet K. Sharma, Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 31

Synthetic talc as a solid base catalyst for condensation of aldehydes and ketones

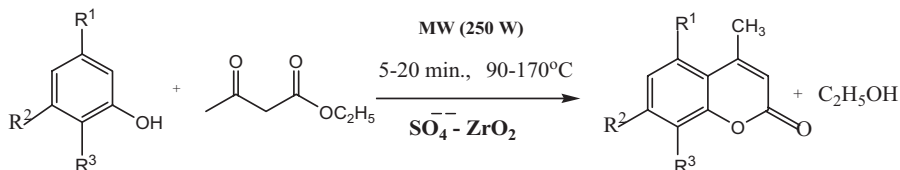
Magnesium organo silicates (MOSs) were synthesized by sol-gel method and used for condensation of aldehydes and ketones. High conversion (86%) of propanal with 95% selectivity of 2-methylpentenal was achieved using dimethyl sulphoxide as a solvent.

**Beena Tyagi, Manish K. Mishra, Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 41

Microwave-assisted solvent free synthesis of hydroxy derivatives of 4-methyl coumarin using nano-crystalline sulfated-zirconia catalyst

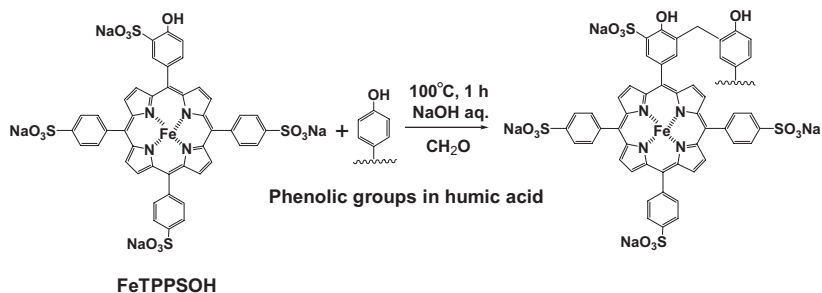
Nano-crystalline sulfated-zirconia catalysts showed good catalytic activity for microwave-assisted solvent free synthesis of hydroxy derivatives of 4-methyl coumarin by Pechmann reaction using activated *m*-hydroxy phenol substrates and ethyl acetoacetate. Less activated phenolic substrates were observed to be inactive under the experimental conditions studied.

**Masami Fukushima**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 47

Oxidative degradation of pentachlorophenol by an iron(III)-porphyrin catalyst bound to humic acid via formaldehyde polycondensation

A biomimetic catalyst, 5-(*p*-hydroxyphenyl)-5,10,15,20-tetrasulfonatophenylporphine iron(III) (FeTPPSOH), was covalently introduced into humic acid via formaldehyde polycondensation. The synthesized catalysts retarded the self-degradation and had higher catalytic activity to the oxidative degradation of pentachlorophenol than the original FeTPPSOH.

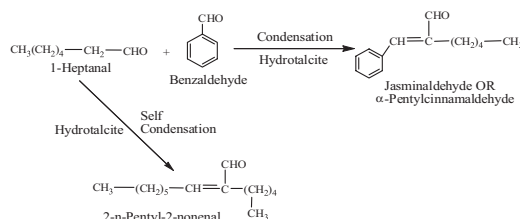


**Sumeet K. Sharma, Parimal A. Parikh,  
Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 55

Eco-friendly synthesis of jasminaldehyde by condensation of 1-heptanal with benzaldehyde using hydrotalcite as a solid base catalyst

The catalytic activity of as-synthesized and activated hydrotalcite ( $[M(II)_{1-x}M(III)_x(OH)_2]^{x+}(CO_3^{2-})_x/n \cdot mH_2O$ ; where  $M(II) = Mg, Ni, Zn$  and  $M(III) = Al$ ) samples of varied divalent metal cations and different divalent to trivalent cations molar ratio was evaluated for the synthesis of jasminaldehyde by solvent free condensation of 1-heptanal with benzaldehyde. The maximum selectivity of jasminaldehyde (86%) with 98% conversion of 1-heptanal was observed using as-synthesized Mg-Al hydrotalcite of Mg/Al molar ratio of 3.5 as a catalyst.

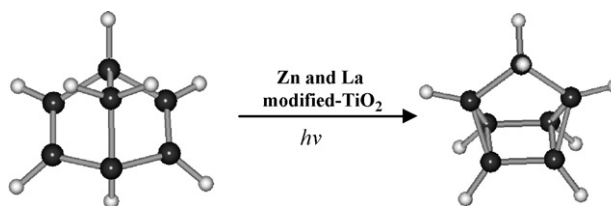


**Ji-Jun Zou, Bin Zhu, Li Wang,  
Xiangwen Zhang, Zhentao Mi**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 63

Zn- and La-modified  $TiO_2$  photocatalysts for the isomerization of norbornadiene to quadricyclane

Zn-doped  $TiO_2$  and Zn-La co-doped  $TiO_2$  was prepared for the photocatalytic isomerization of norbornadiene to quadricyclane. Doping Zn significantly increases the surface-bound OHs of parent particles, whereas doping La reduces the particle to quantum-size. The synergetic effects of surface-bound OHs and quantum-size effect result in significantly high activity.

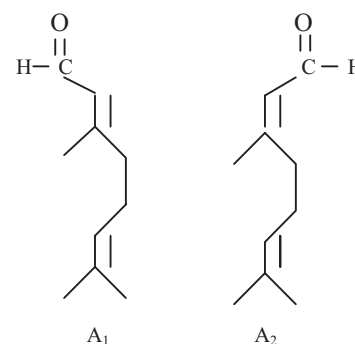


**H. Rojas, G. Borda, J.J. Martínez, J. Valencia,  
P. Reyes**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 70

Liquid phase hydrogenation of citral and intermediaries over Ir/ $TiO_2$ / $SiO_2$  catalysts: Kinetic study

Kinetics of the hydrogenation of citral and its intermediates over Ir/ $TiO_2$ / $SiO_2$  catalysts has been studied. The reaction rate obeys a kinetics represented by the Langmuir-Hinshelwood model. A single site model suggesting the surface reaction as the rate determining step provided the best fit of the experimental data for the hydrogenation of citral and alcohols (geraniol, nerol and citronellol), while a dual site represent the best kinetics for the hydrogenation of citronellal.



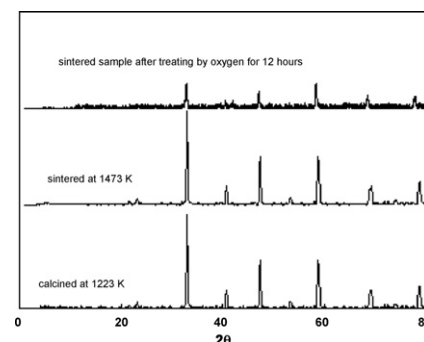
$A_1$ : Citral E.  $A_2$ : Citral Z

**Z. Taheri, K. Nazari, A.A. Safekordi,  
N. Seyed-Matin, R. Ahmadi, N. Esmaeili,  
A. Tofigh**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 79

Oxygen permeation and oxidative coupling of methane in membrane reactor: A new facile synthesis method for selective perovskite catalyst

A new complexation agent ethylene diamine  $N,N,N',N'$ -tetra  $N$ -acetyl diamine (EDTNAD) was successfully used for facile single step preparation of the stable LSCF perovskite,  $La_{0.6}Sr_{0.4}Co_{0.8}Fe_{0.2}O_{3-\delta}$ . The LSCF membrane showed good oxygen permeability based on the bulk diffusion mechanism. OCM reaction using LSCF disk in the atmospheric membrane reactor conducted the process toward 100%  $C_2$  selectivity and high yield (5%) at 1153 K.

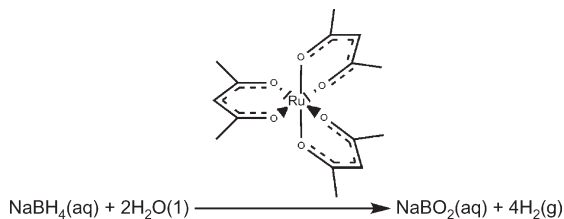


**Ezgi Keçeli, Saim Özkar**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 87

Ruthenium(III) acetylacetonate: A homogeneous catalyst in the hydrolysis of sodium borohydride

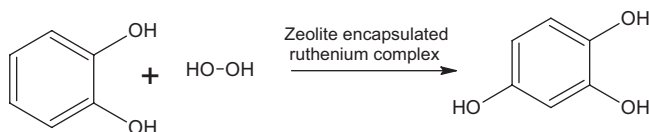
Ruthenium(III) acetylacetonate was employed for the first time as homogeneous catalyst in the hydrolysis of sodium borohydride and found to be highly active catalyst providing 1200 turnovers before deactivation. Poisoning experiments with mercury and trimethylphosphite provide compelling evidence for homogeneous catalyst. Catalytic hydrolysis is first order with respect to both the substrate and catalyst concentration.

**Pearly Sebastian Chittilappilly, N. Sridevi, K. K. Mohammed Yusuff**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 92

Ruthenium complexes of Schiff base ligands as efficient catalysts for catechol–hydrogen peroxide reaction

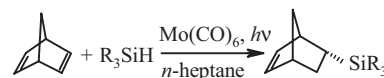
Zeolite Y-encapsulated ruthenium(III) complexes of Schiff bases derived from 3-hydroxyquinoxaline-2-carboxaldehyde and 1,2-phenylenediamine, 2-aminophenol, or 2-aminobenzimidazole (RuYqpd, RuYqap and RuYqab, respectively) and the Schiff bases derived from salicylaldehyde and 1,2-phenylenediamine, 2-aminophenol, or 2-aminobenzimidazole (RuYsalpd, RuYsalap and RuYsalab, respectively) have been prepared and characterized. These complexes except RuYqpd catalyze catechol oxidation by H<sub>2</sub>O<sub>2</sub> selectively to 1,2,4-trihydroxybenzene. A comparative study in terms of initial rates, percentage conversion of the reaction and turn over frequency of the catalysts was done. The reaction is believed to proceed through the formation of Ru(V).

**Magdalena Stosur, Teresa Szymańska-Buzar**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 98

Facile hydrosilylation of norbornadiene by silanes R<sub>3</sub>SiH and R<sub>2</sub>SiH<sub>2</sub> with molybdenum catalysts

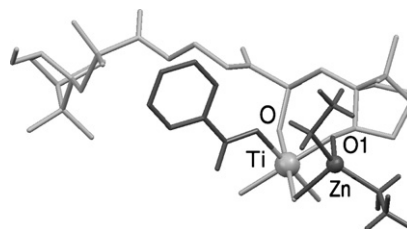
Photochemically activated [Mo(CO)<sub>6</sub>] and [Mo(CO)<sub>4</sub>(η<sup>4</sup>-nbd)] have been demonstrated to be very effective catalysts for hydrosilylation of norbornadiene (nbd) by tertiary (Et<sub>3</sub>SiH, Cl<sub>3</sub>SiH) and secondary (Et<sub>2</sub>SiH<sub>2</sub> and Ph<sub>2</sub>SiH<sub>2</sub>) silanes to give 5-silyl-2-norbornene, which under the same reaction conditions transform in ring-opening metathesis polymerization to unsaturated polymers and to a double hydrosilylation product, 2,6-bis(silyl) norbornane.

**Anna Kozakiewicz, Małgorzata Ullrich, Mirosław Wetniak, Andrzej Wojtczak**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 106

C<sub>2</sub>-symmetrical bis(camphorsulfonamides) as chiral ligands for enantioselective addition of diethylzinc to benzaldehyde

Activity of chiral bis(ketosulfonamides) and bis(hydroxysulfonamides) ligands derived from camphor was determined in the addition of diethylzinc to benzaldehyde in a presence of titanium(IV) isopropoxide. The bis(ketosulfonamide) ligands reveal low enantioselectivity (ee < 12%). The bis(hydroxysulfonamides) reveal much higher asymmetric induction. The best enantiomeric excess (62%) has been observed for bis(hydroxysulfonamide) obtained from 1,3-diaminepropane. Crystal structures have been determined for bis(ketosulfonamide) ligands and bis(hydroxysulfonamide) containing the C<sub>2</sub> bridge.

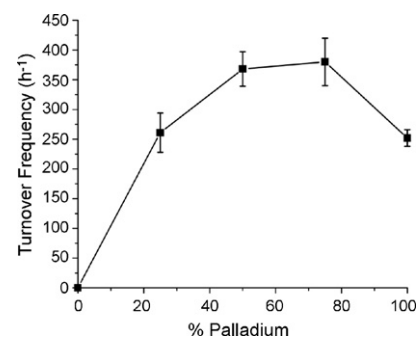


**Priyabrat Dash, Nicole A. Dehm,  
Robert W.J. Scott**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 114

Bimetallic PdAu nanoparticles as hydrogenation catalysts in imidazolium ionic liquids

Bimetallic PdAu nanoparticles stabilized by poly(vinylpyrrolidone) in a [BMIM]PF<sub>6</sub> ionic liquid phase were examined as catalysts for hydrogenation reactions, with nanoparticles with high Pd loadings showing the highest activities for hydrogenation reactions (as shown for the hydrogenation of allyl alcohol).

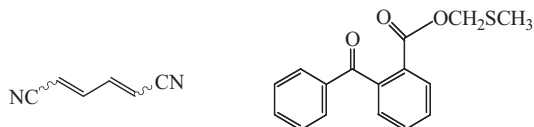


**Kohichi Kashiwagi, Ryoji Sugise,  
Toshihiro Shimakawa, Tuna Matuura,  
Masashi Shirai**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 120

Elucidation of inhibitors in the dimerization of acrylonitrile using [RuCl<sub>2</sub>(DMSO)<sub>4</sub>/CH<sub>3</sub>CH<sub>2</sub>COONa/DMSO/*o*-benzoylbenzoic acid] as catalyst

1,4-Dicyanobuta-1,3-diene and methylthiomethyl *o*-benzoylbenzoate act as inhibitors in the dimerization reaction of acrylonitrile using the novel catalytic system of [RuCl<sub>2</sub>(DMSO)<sub>4</sub>/CH<sub>3</sub>CH<sub>2</sub>COONa/DMSO/*o*-benzoylbenzoic acid].

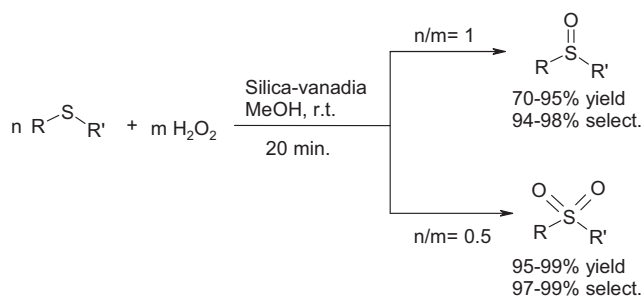


**Francesca Gregori, Ilaria Nobili,  
Franca Bigi, Raimondo Maggi,  
Giovanni Predieri,  
Giovanni Sartori**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 124

Selective oxidation of sulfides to sulfoxides and sulfones using 30% aqueous hydrogen peroxide and silica-vanadia catalyst

A green, efficient and selective approach for the oxidation of sulfides to sulfoxides and sulfones with stoichiometric amount of 30% aq. H<sub>2</sub>O<sub>2</sub> is reported. The reaction is performed in methanol with silica-vanadia as heterogeneous and reusable catalyst.

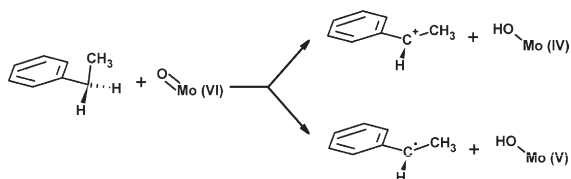


**Maciej Szaleniec, Malgorzata Witko,  
Johann Heider**

*Journal of Molecular Catalysis A: Chemical* 286 (2008) 128

Quantum chemical modelling of the C-H cleavage mechanism in oxidation of ethylbenzene and its derivatives by ethylbenzene dehydrogenase

Ethylbenzene dehydrogenase is an enzyme capable of oxygen-independent stereospecific oxidation of ethylbenzene to (*S*)-1-phenylethanol. It also oxidises a wide range of other alkylaromatic and alkylheterocyclic compounds. The nature of rate-limiting step, formation of either radical or carbocation, is assessed by correlation analysis of kinetic rate constants and Gibbs free energies of formation of both radical and carbocation intermediates calculated on DFT level. The article introduces useful QSAR methodology for investigation of the chemical mechanisms.

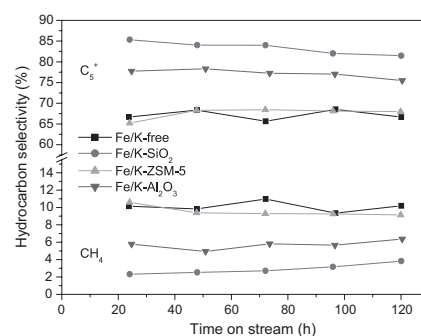


**Guoyan Zhao, Chenghua Zhang,  
Shaodong Qin, Hongwei Xiang, Yongwang Li**

*Journal of Molecular Catalysis A: Chemical* 286  
(2008) 137

Effect of interaction between potassium and structural promoters on Fischer–Tropsch performance in iron-based catalysts

The Fischer–Tropsch synthesis (FTS) performances of iron-based catalysts promoted with/without potassium compounds containing different acidic structural promoters ( $\text{Al}_2\text{O}_3$ ,  $\text{SiO}_2$ , and ZSM-5) were studied in this research. The figure shows the effect of different potassium promoters on hydrocarbon selectivity and the results can be explained from the interaction between potassium and structure promoters, and the spillover of reactants or intermediates from Fe sites to the surfaces of structural promoters.

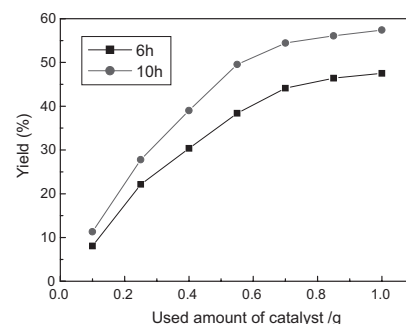


**Baojiao Gao, Delun Kong, Yan Zhang**

*Journal of Molecular Catalysis A: Chemical* 286  
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Preparation and catalytic activity of P4VP–Cu(II) complex supported on silica gel

The catalyst Cu(II)–P4VP/SiO<sub>2</sub> was used in the catalytic oxidation of ethyl benzene to acetophenone by molecular oxygen. The yield of acetophenone is rapidly enhanced with the increase of the used amount of catalyst Cu(II)–P4VP/SiO<sub>2</sub>, indicating its high catalytic activity.



**Hua Xiao, Ruiping Liu, Xu Zhao, Jihui Qu**

*Journal of Molecular Catalysis A: Chemical* 286  
(2008) 149

Enhanced degradation of 2,4-dinitrotoluene by ozonation in the presence of manganese(II) and oxalic acid

In this manuscript, the homogeneous catalyst Mn(II) was investigated, which showed much highly effective for the degradation of DNT by ozone in the presence of oxalic acid. The study revealed a different catalytic mechanism in Mn(II) homogeneous catalytic ozonation of organics through the addition of oxalic acid, which will enrich the research in catalytic ozonation, especially homogeneous catalytic ozonation.

**Dmitry Yu. Murzin, Irina L. Simakova**

*Journal of Molecular Catalysis A: Chemical* 286  
(2008) 156

Kinetic aspects of stereoselectivity in hydrogenation of fatty acids

Analysis of kinetics and *cis/trans* stereoselectivity as a function of reaction parameters (pressure, temperature, conversion) was performed for hydrogenation of fatty acids and their derivatives. A reaction mechanism is proposed, which is consistent with experimental observations. Kinetic parameters are established for hydrogenation of *cis,cis*,9,12 methyl linoleate over Pd/MgO.

