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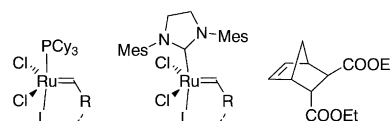
Articles

Sandra Demel, Wolfgang Schoefberger, Christian Slugovc, Franz Stelzer

Journal of Molecular Catalysis A: Chemical 200 (2003) 11

Benchmarking of ruthenium initiators for the ROMP of a norbornedicarboxylic acid ester

The kinetic study of ring-opening metathesis polymerization (ROMP) of a diester functionalised norbornene derivative with a series of Ruthenium benzylidene complexes revealed the applicability of these initiators for well defined polymerization reactions.

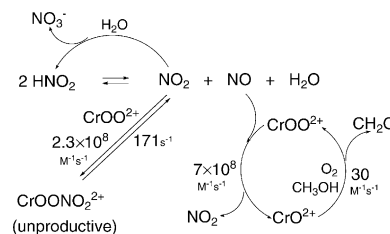


Oleg Pestovsky, Andreja Bakac

Journal of Molecular Catalysis A: Chemical 200 (2003) 21

Superoxometal-catalyzed co-oxidation of alcohols and nitrous acid with molecular oxygen

$\text{Cr}_{\text{aq}}\text{OO}^{2+}$ catalyzes the co-oxidation of alcohols and nitrous acid with molecular oxygen, $\text{CH}_3\text{OH} + \text{HNO}_2 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{NO}_3^- + \text{H}_2\text{O} + \text{H}^+$. The mechanism features the disproportionation of nitrous acid to NO and NO_2 , reduction of $\text{Cr}_{\text{aq}}\text{OO}^{2+}$ with NO to generate $\text{Cr}_{\text{aq}}\text{O}^{2+}$, and oxidation of the substrate by $\text{Cr}_{\text{aq}}\text{O}^{2+}$ in a step that regenerates the catalyst.

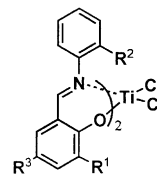


Rieko Furuyama, Junji Saito, Sei-ichi Ishii, Makoto Mitani, Shigekazu Matsui, Yasushi Tohi, Haruyuki Makio, Naoto Matsukawa, Hidetsugu Tanaka, Terunori Fujita

Journal of Molecular Catalysis A: Chemical 200 (2003) 31

Ethylene and propylene polymerization behavior of a series of bis(phenoxy-imine)-titanium complexes

A series of bis(phenoxy-imine)Ti complexes were investigated as ethylene and propylene polymerization catalysts. The steric bulk of the substituent *ortho* to the phenoxy-oxygen is shown to be fundamental to obtaining high catalytic performance. With the complexes having sterically-hindered substituents *ortho* to the phenoxy-oxygen, a high ethylene polymerization activity, 3240kg/mol-cat h, and a high syndiospecificity, *rrrr* 83.7%, was achieved.



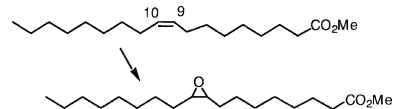
Complexes	R ¹	R ²	R ³
1	H	H	H
2	Me	H	H
3	^t Bu	H	H
4	SiMe ₃	H	H
5	^t Bu	Me	H
6	^t Bu	ⁱ Pr	H
7	^t Bu	H	Me
8	^t Bu	H	^t Bu

Abdillahi Omar Bouh, James H. Espenson

Journal of Molecular Catalysis A: Chemical
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Epoxidation reactions with urea–hydrogen peroxide catalyzed by methyltrioxorhenium(VII) on niobia

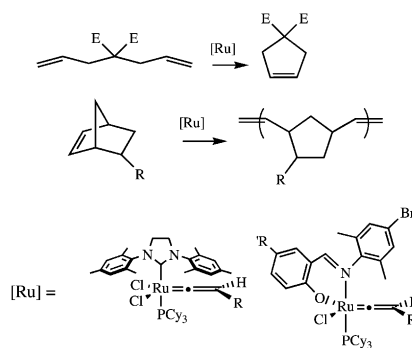
Methyl oleate and other soybean oils are epoxidized by urea–hydrogen peroxide with MeReO_3 supported on niobia as the catalyst.



Tom Opstal, Francis Verpoort

Journal of Molecular Catalysis A: Chemical
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Easily accessible and robust olefin–metathesis catalysts based on ruthenium vinylidene complexes

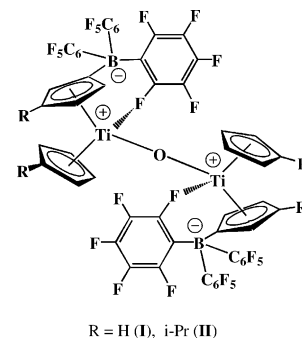


V.V. Burlakov, A.V. Letov, P. Arndt, W. Baumann, A. Spannenberg, Ch. Fischer, L.I. Strunkina, M.Kh. Minacheva, Ya.S. Vygodskii, U. Rosenthal, V.B. Shur

Journal of Molecular Catalysis A: Chemical
200 (2003) 63

Zwitterionic titanoxanes $\{\text{Cp}[\eta^5\text{-C}_5\text{H}_4\text{B}(\text{C}_6\text{F}_5)_3]\text{Ti}\}_2\text{O}$ and $\{(\eta^5\text{-}i\text{-PrC}_5\text{H}_4)[\eta^5\text{-}1,3\text{-}i\text{-PrC}_5\text{H}_3\text{B}(\text{C}_6\text{F}_5)_3]\text{Ti}\}_2\text{O}$ as catalysts for cationic ring-opening polymerization

Zwitterionic titanoxanes (**I**) and (**II**), which contain two positively charged Ti(IV) centres in the molecule, are able to catalyse the ring-opening polymerization of ϵ -caprolactone, tetrahydrofuran and propylene oxide. The reactions found are the first examples of catalysis of the cationic ring-opening polymerization by zwitterionic metallocenes of the group IVB metals.

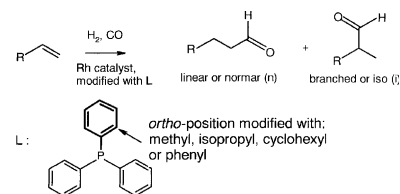


Helena Riihimäki, Pekka Suomalainen, Heidi K. Reinius, Johanna Suutari, Sirpa Jääskeläinen, A.O.I. Krause, Tapani A. Pakkanen, Jouni T. Pursiainen

Journal of Molecular Catalysis A: Chemical
200 (2003) 69

o-Alkyl-substituted aromatic phosphanes for hydroformylation studies: synthesis, spectroscopic characterization and ab initio investigations

o-Alkyl-substituted arylphosphane ligands were synthesized and tested in Rh-based hydroformylation of propene and 1-hexene in order to study their effects on *iso*-selectivity and activity. The bulkiness of the ligands was varied by the size of the *o*-substituent. The *o*-substituted arylphosphanes provided higher *iso*-selectivity compared to widely used ligand triphenylphosphane.

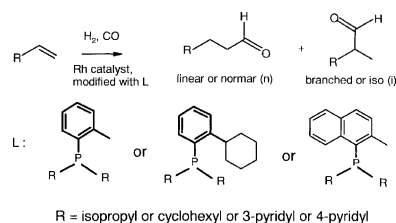


**Helena Riihimäki, Teija Kangas,
Pekka Suomalainen, Heidi K. Reinius,
Sirpa Jääskeläinen, Matti Haukka,
A.O.I. Krause, Tapani A. Pakkanen,
Jouni T. Pурсiainen**

Journal of Molecular Catalysis A: Chemical
200 (2003) 81

Synthesis of new *o*-alkyl substituted arylalkylphosphanes: study of their molecular structure and influence on rhodium-catalyzed propene and 1-hexene hydroformylation

o-Alkyl-substituted arylalkylphosphane ligands were synthesized and tested in Rh-based hydroformylation of propene and 1-hexene in order to study their effects on *iso*-selectivity and activity. The steric and electronic properties of phosphanes were concomitantly modified by combining the previously approved sterically crowded *o*-alkyl-substituted aryl groups with better σ -donor groups, isopropyls or cyclohexyls. Additionally, the electronic modification was done with pyridyl groups.

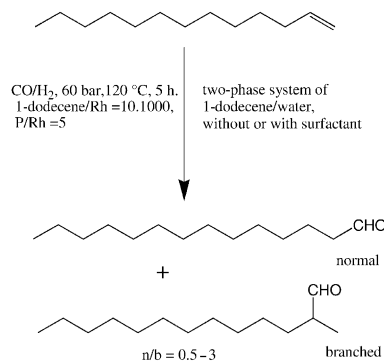


**E. Paetzold, G. Oehme, C. Fischer,
M. Frank**

Journal of Molecular Catalysis A: Chemical
200 (2003) 95

Phosphinoethyl-sulfonatoalkylthioethers and diphenyl-*o*-sulfonatoalkyl-phosphines as ligands and polyoxyethylene-polyoxypropylene-polyoxyethylene triblock co-polymers as promoters in the rhodium-catalyzed hydroformylation of 1-dodecene in aqueous two-phase systems

The hydroformylation of 1-dodecene was investigated with new water-soluble phosphine rhodium complexes in two-phase systems with or without surfactants. The recycling of the catalyst in the water phase was achieved without detergent or in presence of small amounts of triblock co-polymers at room temperature by phase separation. The substrate/rhodium ratio was 10.000 and the TON could be increased with triblock co-polymers up to 65.000.

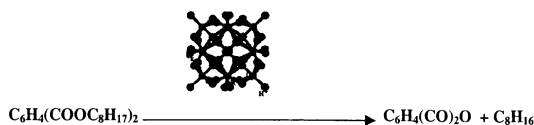


**M. Arabi, M. Mohammadpour Amini,
M. Abedini, A. Nemati, M. Alizadeh**

Journal of Molecular Catalysis A: Chemical
200 (2003) 105

Esterification of phthalic anhydride with 1-butanol and 2-ethylhexanol catalyzed by heteropolyacids

Esterification of phthalic anhydride and ester decomposition of dioctyl phthalate in presence of Keggin, Wells-Dawson and Preyssler type heteropolyacids has been investigated. A complete conversion of phthalic anhydride to dioctyl phthalate and dibutyl phthalate are achieved in 2h in presence of molybdenum substituted Preyssler heteropolyacid. In the decomposition of dioctyl phthalate, 2-ethylhexene is formed in quantitative yield.

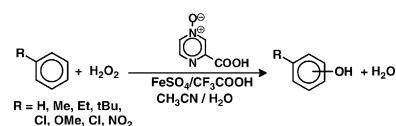


**Daniele Bianchi, Marcello Bertoli,
Roberto Tassinari, Marco Ricci,
Rodolfo Vignola**

Journal of Molecular Catalysis A: Chemical
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Direct synthesis of phenols by iron-catalyzed biphasic oxidation of aromatic hydrocarbons with hydrogen peroxide

The hydroxylation of a series of aromatic hydrocarbons with hydrogen peroxide, catalyzed by iron complexes with pyrazine-3-carboxylic acid *N*-oxide, was investigated, operating in a biphasic reaction medium. In most cases, the new catalysts showed a good selectivity to give the corresponding phenols, and was reused in several consecutive cycles without any appreciable loss of activity.

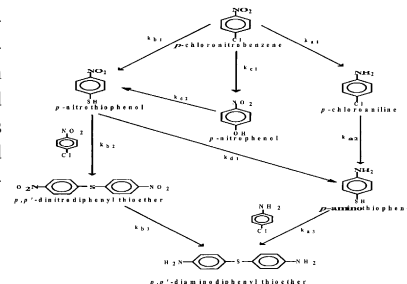


Ganapati D. Yadav, Yogeeta B. Jadhav, Sonali Sengupta

Journal of Molecular Catalysis A: Chemical 200 (2003) 117

Selectivity engineered phase transfer catalysis in the synthesis of fine chemicals: reactions of *p*-chloronitrobenzene with sodium sulphide

Selectivity engineered phase transfer catalysis in the synthesis of fine chemicals: reactions of *p*-chloronitrobenzene with sodium sulphide. A variety of useful products could be produced by manipulating the conditions under the theme of selectivity engineered phase transfer catalysed reaction of *p*-chloronitrobenzene and sodium sulphide.

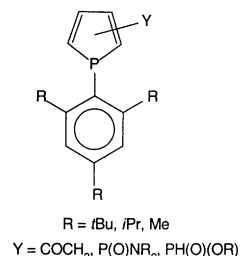


György Keglevich, Tamás Kégl, Tungalag Chuluunbaatar, Beáta Dajka, Péter Mátyus, Balázs Balogh, László Kollár

Journal of Molecular Catalysis A: Chemical 200 (2003) 131

Hydroformylation of styrene in the presence of rhodium-2,4,6-trialkylphenyl-phosphole in situ catalytic systems

P-arylphospholes of high aromaticity were used in rhodium-catalysed hydroformylation. The results obtained by the systematic variation of the aryl substituent were rationalised on the basis of ³¹P NMR and density functional calculations.

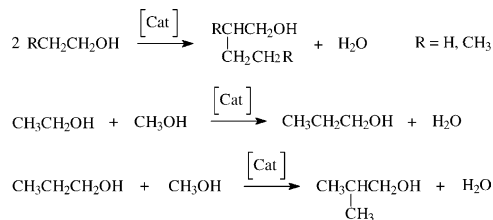


Carlo Carlini, Marco Di Girolamo, Alessandro Macinai, Mario Marchionna, Marilena Noviello, Anna Maria Raspolli Galletti, Glauco Sbrana

Journal of Molecular Catalysis A: Chemical 200 (2003) 137

Selective synthesis of isobutanol by means of the Guerbet reaction. Part 2. Reaction of methanol/ethanol and methanol/ethanol/*n*-propanol mixtures over copper based/MeONa catalytic systems

The isobutanol synthesis by the Guerbet condensation of methanol with ethanol and/or *n*-propanol was studied in the presence of sodium methoxide and copper based catalytic systems. The effect of reaction parameters (temperature, catalyst formulation, alcohols mixture composition, etc.) on isobutanol yield was investigated in order to optimize process performances.

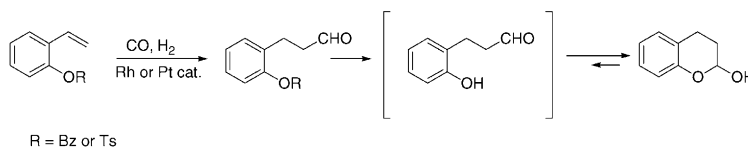


C. Botteghi, S. Paganelli, F. Moratti, M. Marchetti, R. Lazzaroni, R. Settambolo, O. Piccolo

Journal of Molecular Catalysis A: Chemical 200 (2003) 147

Synthesis of 2-chromanol by hydroformylation of 2-hydroxystyrene derivatives

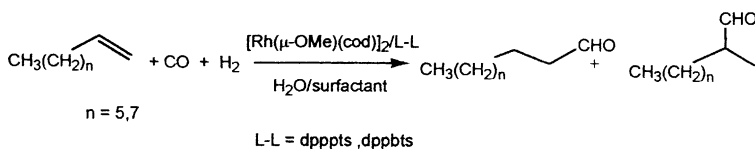
2-Benzyloxy- and 2-tosyloxystyrene were hydroformylated under different reaction conditions with the aim to obtain the corresponding linear aldehydes, valuable intermediates to 2-chromanol, a structural moiety present in several interesting therapeutically active molecules.



**Marta Giménez-Pedrés, Ali Aghmiz,
Carmen Claver, Anna M. Masdeu-Bultó,
Denis Sinou**

Journal of Molecular Catalysis A: Chemical
200 (2003) 157

Micellar effect in hydroformylation of high olefin catalysed by water-soluble rhodium complexes associated with sulfonated diphosphines

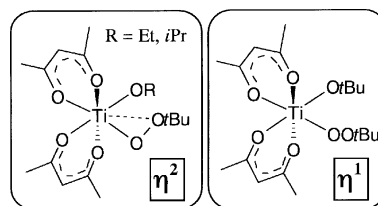


D.E. Babushkin, E.P. Talsi

Journal of Molecular Catalysis A: Chemical
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Formation, solution structure and reactivity of alkylperoxo complexes of titanium

The following titanium alkylperoxo complexes were characterized in situ: $\text{Ti}(\eta^2\text{-OOtBu})_n(\text{OiPr})_{4-n}$ ($n = 1-4$), $[(i\text{PrO})_3\text{Ti}(\mu\text{-OiPr})_2\text{-Ti}(\text{OiPr})_2(\eta^2\text{-OOtBu})]$, $[(\eta^2\text{-OOtBu})(i\text{PrO})_2\text{-Ti}(\mu\text{-OiPr})_2\text{-Ti}(\text{OiPr})_2(\eta^2\text{-OOtBu})]$, $\text{Ti}(\text{LL})_2(\text{OR})(\eta^2\text{-OOtBu})$, $\text{Ti}(\text{LL})_2(\eta^2\text{-OOtBu})_2$ and $\text{Ti}(\text{LL})_2(\text{ORtBu})(\eta^1\text{-OOtBu})$, where $R = \text{Et, } i\text{Pr}$; HLL = acetylacetonate, dipivaloylmethane.

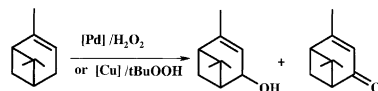


**Badia Ait Allal, Larbi El Firdoussi,
Smail Allaoud, Abdallah Karim,
Yves Castanet, André Mortreux**

Journal of Molecular Catalysis A: Chemical
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Catalytic oxidation of α -pinene by transition metal using *t*-butyl hydroperoxide and hydrogen peroxide

According to the catalytic system, the oxidation of α -pinene by *t*BuOOH can be directed toward the selective formation of the allylic ketone (Cu salts) or the allylic alcohol (Pd).

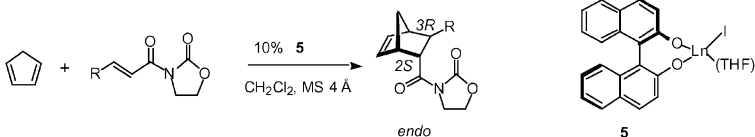


**Jacqueline Collin, Fabien Carrée,
Nicolas Giuseppone, Isabel Santos**

Journal of Molecular Catalysis A: Chemical
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(*R*)-bis-Binaphthoxy iodo lanthanides as catalysts for Diels–Alder reactions

Bidentate lanthanide iodo binaphthoxides **5** (Ln: Yb, Sm, La) have been prepared by reaction of the bispotassium salt of (*R*)-binaphthol with lanthanide triiodides, and investigated as enantioselective catalysts for Diels–Alder reactions.

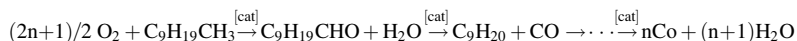


Melvin Keith Carter

Journal of Molecular Catalysis A: Chemical
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Catalytic air oxidation of ambient temperature hydrocarbons

Catalytic air oxidation of the aliphatic hydrocarbons was conducted at ambient temperature, using novel iron catalysts, producing essentially quantitative amounts of carbon monoxide and water



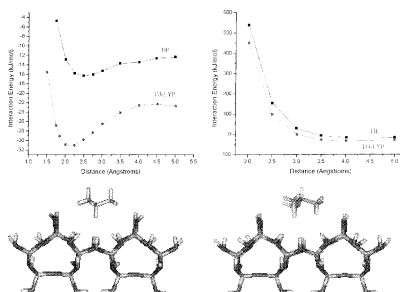
The catalysts were designed, prepared, applied and analyzed, and the indicated catalytic reaction mechanisms were discussed.

**L.A. García-Serrano,
C.A. Flores-Sandoval, I.P. Zaragoza**

Journal of Molecular Catalysis A: Chemical
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Theoretical study of the adsorption of isobutane over H-mordenite zeolite by ab initio and DFT methods

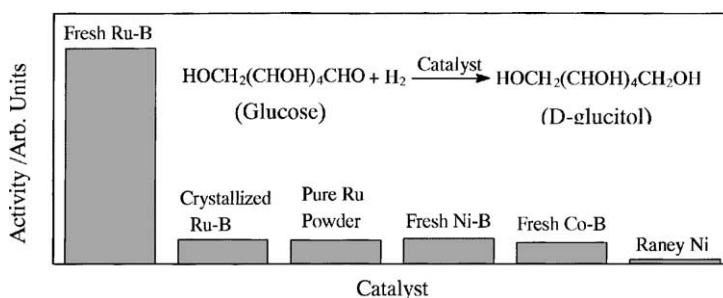
Steric hindrance and adsorption effect were observed by interaction energy calculation between the isobutane molecule and acid site of H-mordenite.



**Haibing Guo, Hexing Li, Jian Zhu,
Wanhua Ye, Minghua Qiao, Weilin Dai**

Journal of Molecular Catalysis A: Chemical
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Liquid phase glucose hydrogenation to D-glucitol over an ultrafine Ru-B amorphous alloy catalyst

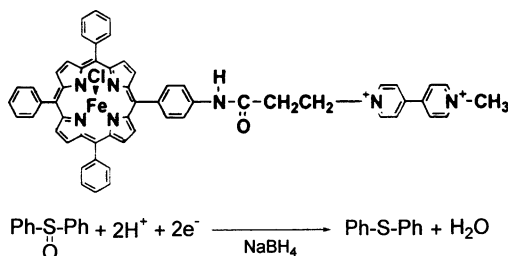


**Hiroaki Koga, Takeyuki Arai,
Taisuke Hamada, Shigeyoshi Sakaki**

Journal of Molecular Catalysis A: Chemical
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Application of metalloporphyrins and methylviologen-pendent iron porphyrin to reduction of diphenylsulfoxide

Methylviologen-pendent iron porphyrin much more efficiently catalyzes two-electron reduction of diphenylsulfoxide to diphenylsulfide with NaBH_4 than usual metalloporphyrins.

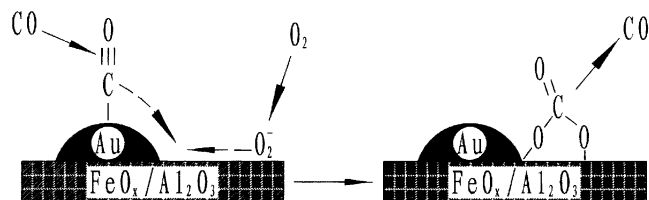


**Donghui Wang, Zhengping Hao,
Daiyun Cheng, Xicheng Shi, Chun Hu**

Journal of Molecular Catalysis A: Chemical
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Influence of pretreatment conditions on low-temperature CO oxidation over Au/MO_x/Al₂O₃ catalysts

The composite oxide FeO_x/Al₂O₃ supported gold catalyst showed very good performance for the low-temperature CO oxidation.

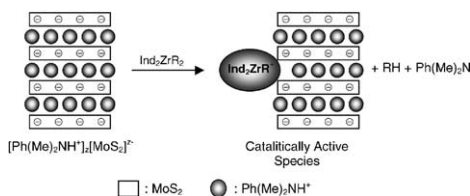


**Satoru Yamada, Akihiro Yano,
Morihiro Sato, Takahito Itoh**

Journal of Molecular Catalysis A: Chemical
200 (2003) 239

Effect of "topotactic" reduction product of molybdenum disulfide on catalytic activity of metallocene catalyst for olefin polymerization

In ethylene polymerization, addition of *N,N*-dimethylanilinium ion (Ph(Me)₂NH⁺) intercalated MoS₂ as a cocatalyst to Ind₂ZrCl₂/Et₃Al was found to improve significantly the catalytic activity per mmol of Ind₂ZrCl₂. It was proposed that neutral dialkylmetallocene was protonated by Ph(Me)₂NH⁺ in the interlayer space of MoS₂, especially on the edge of the layered structure of MoS₂, to form the cationic monoalkylmetallocene as an active species with liberation of a neutral amine.

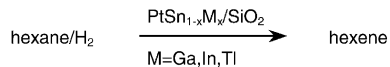


**Narcís Homs, Jordi Llorca,
Montserrat Riera, Jordi Jolis,
José-Luis G. Fierro, Joaquim Sales,
Pilar Ramírez de la Piscina**

Journal of Molecular Catalysis A: Chemical
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Silica-supported PtSn alloy doped with Ga, In or, Tl. Characterization and catalytic behaviour in *n*-hexane dehydrogenation

Silica-supported PtSn_{1-x}M_x particles were prepared from monometallic precursors, trimetallic particles showed a high selectivity to dehydrogenation products in the *n*-hexane reactions. The incorporation of a group 13 metal into PtSn alloy produced an electronic effect on platinum, which was determined by X-ray photoelectron spectroscopy (XPS) and CO chemisorption experiments followed by FT-IR.

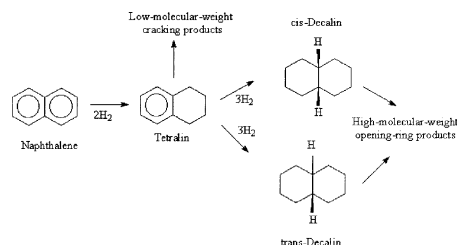


**S. Albertazzi, R. Ganzerla, C. Gobbi,
M. Lenarda, M. Mandreoli, E. Salatelli,
P. Savini, L. Storaro, A. Vaccari**

Journal of Molecular Catalysis A: Chemical
200 (2003) 261

Hydrogenation of naphthalene on noble-metal-containing mesoporous MCM-41 aluminosilicates

Catalysts containing 1 wt.% of noble-metal inside MCM-41 framework were investigated in the hydrogenation of naphthalene. While at atmospheric pressure only Rh and Pd were slightly active, in the tests performed at 6.0 MPa the catalytic activity grew, exhibiting the following order: Pt > Rh >> Pd >>> Ru ≈ Ir. All the catalysts required large H₂ excess and showed low thio-tolerance.



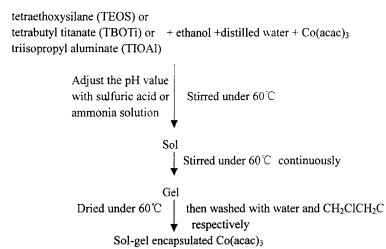
**Qiuyi Hu, Jiquan Zhao, Yanji Wang,
Lingdi Zhu, Mengqing Li, Guohua Li,
Yang Wang, Fengyan Ge**

Journal of Molecular Catalysis A: Chemical
200 (2003) 271

Sol-gel encapsulated cobalt(III) acetylacetonate for air oxidation of penicillin derivatives

$\text{Co}(\text{acac})_3$ was encapsulated physically into SiO_2 , TiO_2 or Al_2O_3 matrix by sol-gel method (Scheme 1).

They were used to catalyze the air oxidation of penicillin derivatives to corresponding sulfoxides. They are leach proof and can be recycled in more than 15 runs with hardly any loss of activity. The conversion of PGPMB was 98.8% and the selectivity to PGPMBO was 100% (Scheme 2).

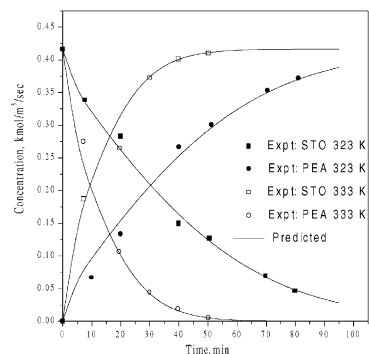


**C.V. Rode, M.M. Telkar, R. Jaganathan,
R.V. Chaudhari**

Journal of Molecular Catalysis A: Chemical
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Reaction kinetics of the selective liquid phase hydrogenation of styrene oxide to β -phenethyl alcohol

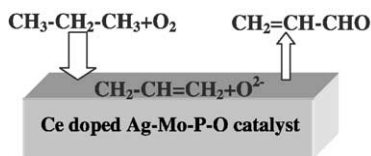
An inhibition effect of both hydrogen (>3 MPa) and styrene oxide (>0.5 kmol/m^3) was observed in the kinetic study of hydrogenation of styrene oxide to β -phenethyl alcohol. A Langmuir-Hinshelwood rate equation has been verified under integral reactor conditions.



**Xin Zhang, Hui-lin Wan,
Wei-zheng Weng, Xiao-dong Yi**

Journal of Molecular Catalysis A: Chemical
200 (2003) 291

Effect of promoter Ce on silver-molybdenum-phosphate catalysts for selective oxidation of propane to acrolein

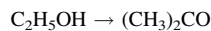


Mohamed Mokhtar Mohamed

Journal of Molecular Catalysis A: Chemical
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Catalytic properties of Fe ion-exchanged mordenite toward the ethanol transformation: influence of the methods of preparation

The exceptional transformation of ethanol (two carbon atoms) into acetone (three carbon atoms) has been taken place on Fe/mordenite catalysts at high Fe contents (100 wt%). This was achieved at the expense of acetaldehyde product that was further oxidized to acetic acid forming iron acetate, which eventually decompose at 400°C into iron carbonate and acetone. The probability of forming iron acetate was emphasized through the existed and rather confirmed Fe^{2+} components.

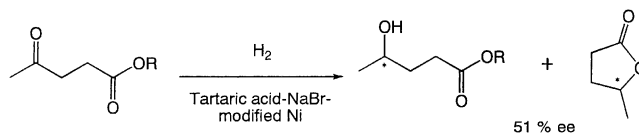


**Tsutomu Osawa, Eri Mieno,
Tadao Harada, Osamu Takayasu**

Journal of Molecular Catalysis A: Chemical
200 (2003) 315

Study of the parameters controlling the enantio-differentiating ability of asymmetrically modified solid catalysts for the hydrogenation of γ -ketoesters

The enantio-differentiating hydrogenation of γ -ketoesters was carried out over asymmetrically modified solid catalysts. The optimal amount of NaBr in the modification solution strongly depended on the nickel catalyst precursor. The addition of an appropriate amount of carboxylic acid to the reaction media increased the enantiomer excess (ee) of the hydrogenated products.



**Nora I. Mäkelä-Vaarne,
David G. Nicholson,
Astrid Lund Ramstad**

Journal of Molecular Catalysis A: Chemical
200 (2003) 323

Supported metallocene catalysts—interactions of $(n\text{-BuCp})_2\text{HfCl}_2$ with methylaluminoxane and silica

The species on supported olefin polymerisation catalysts consisting of $(n\text{-BuCp})_2\text{HfCl}_2$, methylaluminoxane and dehydroxylated silica were identified by EXAFS and UV-Vis spectroscopies.

