

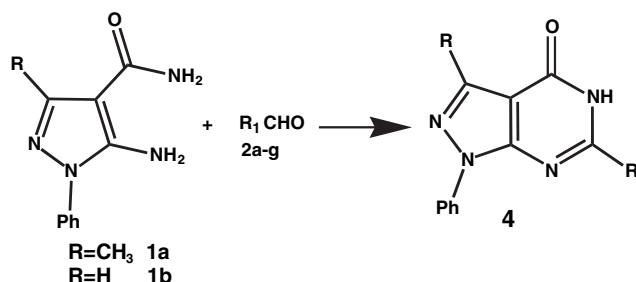
Contents

Articles

**Majid M. Heravi, Radineh Motamedi,
Nasim Seifi, Fatemeh F. Bamoharram**

*Journal of Molecular Catalysis A: Chemical 249
(2006) 1*

Catalytic synthesis of 6-aryl-1H-pyrazolo[3,4-d]pyrimidin-4[5H]-ones by heteropolyacid: $H_{14}[NaP_5W_{30}O_{110}]$ and $H_3PW_{12}O_{40}$

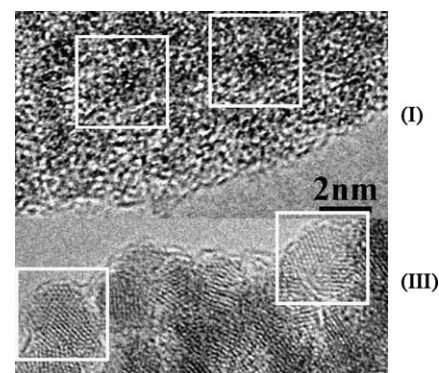


Vladimir P. Oleshko

*Journal of Molecular Catalysis A: Chemical 249
(2006) 4*

Aperiodic core structures of Pd and Pt giant clusters chemically stabilized with diphenyl phosphide ligands

Atomic scale structures of “giant” clusters $[Pd_2(PPh_2)_4]_n$ (**I**) and $[Pt(PPh_2)_4]_n$ (**II**) ($n \cong 6-10$) and $Pd_{\sim 561}Phen_{\sim 60}(OAc)_{\sim 180}$ (**III**) have been investigated by HRTEM and integrated AEM. For (**I**) and (**II**), with 1.5–1.6 nm cores, the structure was found aperiodic. 2.4 nm Pd cores of (**III**) revealed fcc lattice fringes. The differences suggest a ligand induced metal-to-molecular (non-crystalline) state transformation in (**I**) and (**II**).

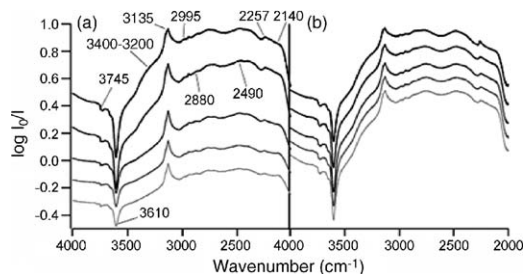


**Dongmei Zhao, Hanna Härelind Ingelsten,
Magnus Skoglundh, Anders Palmqvist**

*Journal of Molecular Catalysis A: Chemical 249
(2006) 13*

Catalytic and mechanistic study of lean NO_2 reduction by isobutane and propane over HZSM-5

The selective catalytic reduction (SCR) of NO_2 by two saturated hydrocarbons, propane and isobutane, has been investigated over acidic zeolite HZSM-5. In situ DRIFT step-response experiments with NO_2 and isobutane show formation of surface bound NO^+ , isocyanate, unsaturated hydrocarbons and amine species. The NO^+ species seems to play an important role in the reduction of NO_2 probably by reacting with alkenes formed from carbenium ion adsorbates.

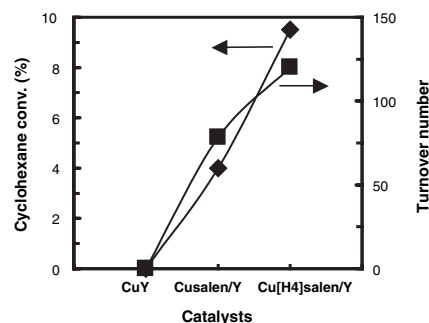


Chun Jin, Weibin Fan, Yinjuan Jia, Binbin Fan, Jinghong Ma, Ruifeng Li

Journal of Molecular Catalysis A: Chemical 249 (2006) 23

Encapsulation of transition metal tetrahydro-Schiff base complexes in zeolite Y and their catalytic properties for the oxidation of cycloalkanes

A variety of transition metal (M=Cu, Co, Fe and Mn) tetrahydro-Schiff base complexes (Schiff=salen, salpn and salicyhexen) have been encapsulated in zeolite Y with flexible ligand method for the first time. The prepared M-[H₄]Schiff/Y catalysts such as Cu-[H₄]salen/Y show much higher conversion in the oxidation of cyclohexane than the corresponding M-Schiff analogues encapsulated in zeolite Y as a result of the incorporation of larger amounts and the stronger oxidation ability of tetrahydro-Schiff base complexes than Schiff base complexes. In addition, M-[H₄]Schiff/Y catalysts are also active for the oxidation of other cycloalkanes.

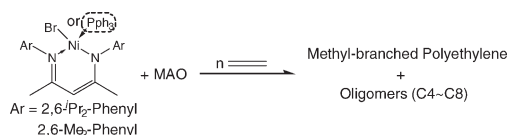


Junkai Zhang, Zhuofeng Ke, Feng Bao, Jieming Long, Haiyang Gao, Fangming Zhu, Qing Wu

Journal of Molecular Catalysis A: Chemical 249 (2006) 31

Ethylene polymerization and oligomerization catalyzed by bulky β-diketiminato Ni(II) and β-diimine Ni(II) complexes/methylaluminoxane systems

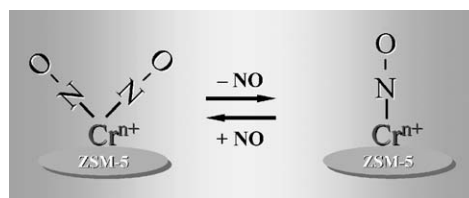
β-Diketiminato Ni(II) complexes/MAO systems catalyzed ethylene polymerization are characterized by simultaneous oligomerization. The obtained ethylene polymers are basically methyl-branched, even if the polymerizations were carried out at higher temperature. Results show that the in-chain migration of Ni(II) center were restrained in β-diketiminato Ni(II)/MAO system.



Mihail Mihaylov, Anna Penkova, Konstantin Hadjiivanov, Marco Daturi

Journal of Molecular Catalysis A: Chemical 249 (2006) 40

Chromium nitrosyl complexes in Cr-ZSM-5: An FTIR spectroscopic study

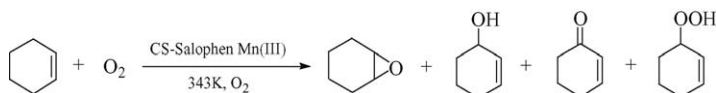


Jinhui Tong, Yan Zhang, Zhen Li, Chungu Xia

Journal of Molecular Catalysis A: Chemical 249 (2006) 47

Highly effective catalysts of natural polymer supported Salophen Mn(III) complexes for aerobic oxidation of cyclohexene

Three chitosan (abbreviated as CS) supported Salophen Mn(III) complexes were prepared in a simple way and characterized by FT-IR and XPS. Their abilities to catalyze allylic oxidation of cyclohexene with oxygen in the absence of solvents or reducing agents were studied. Under reaction conditions of 343 K and ambient pressure of O₂, using CS-Salophen Mn(III) complex as catalyst, 11.03 × 10⁴ turnover numbers was obtained, which was about 44 times as large as that by unsupported Salophen Mn(III) complex.

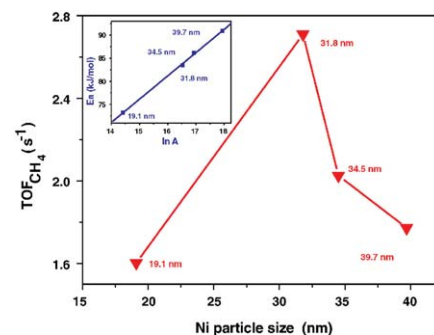


**Yuehua Cui, Hengyong Xu, Qingjie Ge,
Yuzhong Wang, Shoufu Hou, Wenzhao Li**

Journal of Molecular Catalysis A: Chemical 249 (2006) 53

Structure sensitive dissociation of CH₄ on Ni/α-Al₂O₃; Ni nano-scale particles linearly compensate the E_a and ln A for the CH₄ pulse kinetics

This work found that the CH₄ dissociation on Ni particles is a structure sensitive reaction due to the “mountain” shape of the plot of TOF of CH₄ dissociation versus the Ni particle size in the CH₄ pulse through the Ni/α-Al₂O₃. It was also found that E_a and ln A are linear dependence on the Ni particle size of Ni/α-Al₂O₃ and the presence of the compensation effect in the CH₄ dissociation reaction.

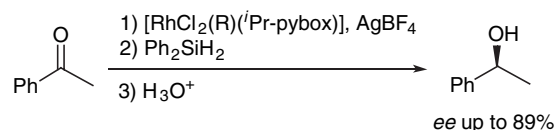


Darío Cuervo, M. Pilar Gamasa, José Gimeno

Journal of Molecular Catalysis A: Chemical 249 (2006) 60

Rhodium(III) complexes containing the ligand 2,6-bis[4'-(S)-isopropylloxazolin-2'-yl]pyridine ((S,S)-iPr-pybox): Efficient catalysts for asymmetric hydrosilylation of acetophenone

The novel dinuclear complex [Rh₂(μ-Cl)₂{(E)-C(Me)=CH(Ph)}₂(iPr-pybox)₂][BF₄]₂ and several mononuclear rhodium(III) complexes [RhCl₂(R)(iPr-pybox)] (R=acyl, allyl, allenyl, alkenyl), containing the enantiopure ligand (S,S)-iPr-pybox, have been examined as catalysts in the asymmetric reduction of acetophenone via the hydrosilylation reaction with diphenylsilane.

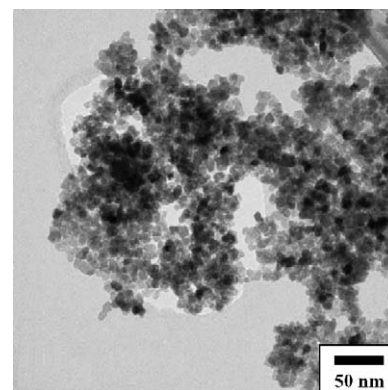


KunWei Li, Hao Wang, Hui Yan

Journal of Molecular Catalysis A: Chemical 249 (2006) 65

Hydrothermal preparation and photocatalytic properties of Y₂Sn₂O₇ nanocrystals

Nanosized Y₂Sn₂O₇ powder photocatalysts with different particle sizes were synthesized through the low temperature hydrothermal method by using different organic agents. Photocatalytic measurements showed Y₂Sn₂O₇ nanocrystals with about 10 nm particle sizes possess superior photocatalytic properties in water purification and may find potential application in related fields.

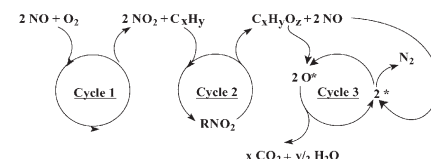


**Cyril Thomas, Olivier Gorce, Françoise Villain,
Gérald Djéga-Mariadassou**

Journal of Molecular Catalysis A: Chemical 249 (2006) 71

Influence of the nature of the noble metal on the lean C₃H₆-assisted decomposition of NO on Ce_{0.68}Zr_{0.32}O₂-supported catalysts

Lean deNO_x assisted by C₃H₆ shows that the order of reactivity of PGMs supported on Ce_{0.68}Zr_{0.32}O₂ is: Pd ≫ Pt ≳ Rh. The selectivity to N₂ of these catalysts is much higher than those reported in the literature for zero-valent PGMs suggesting the existence of a deNO_x mechanism different from that occurring on zero-valent PGMs.

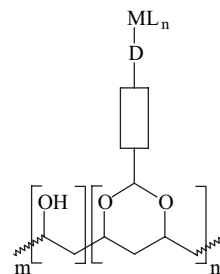


Martin Ahlmann, Olaf Walter, Melany Frank, Wilhelm Habicht

Journal of Molecular Catalysis A: Chemical 249 (2006) 80

Phosphino-functionalised acetals of polyvinyl alcohol as the matrix for the immobilisation of Rh-based pre-catalysts for interfacial catalysis

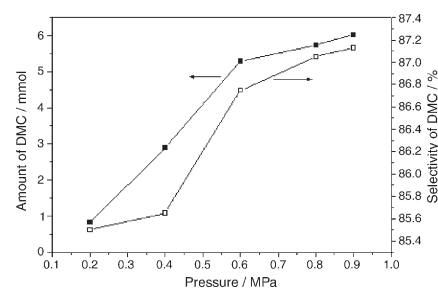
Phosphino functionalisation is introduced in polyvinylalcohol (PVA) by a trans-acetalation reaction, high acetalation degrees can be reached. By complexation of the phosphino groups [Rh]-modified polymers are obtained. The use of the [Rh]-modified polymers as pre-catalysts is presented. Recycling experiments were performed and the catalyst rest state on the polymer was identified. The results show that PVA may be a suitable material for the immobilisation of molecular catalysts forming stable layers on an inorganic support with a possible application in interfacial catalysis.


X.L. Wu, Y.Z. Meng, M. Xiao, Y.X. Lu

Journal of Molecular Catalysis A: Chemical 249 (2006) 93

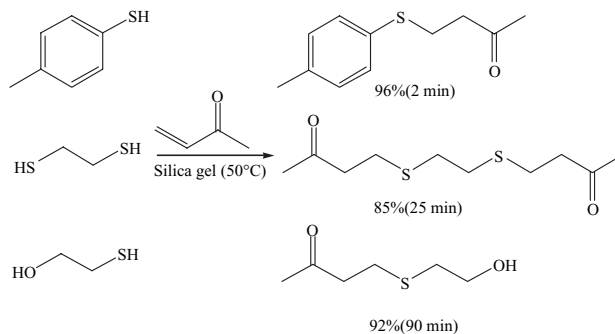
Direct synthesis of dimethyl carbonate (DMC) using Cu-Ni/VSO as catalyst

The catalytic effects of synthesized Cu-Ni/VSO catalysts on the synthesis of dimethyl carbonate (DMC) from CO₂ and CH₃OH were investigated. DRIFT spectra of the catalyst showed that CO₂ and CH₃OH were activated effectively by the catalysts, as evidenced by the high DMC yield and selectivity of CH₃OH.


Habib Firouzabadi, Nasser Iranpoor, Maasoumeh Jafarpour, Arash Ghaderi

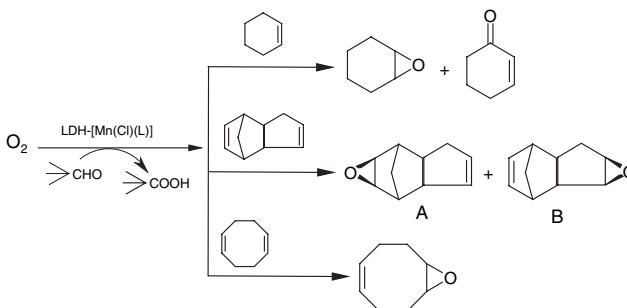
Journal of Molecular Catalysis A: Chemical 249 (2006) 98

Silica gel catalyzed highly selective C-S bond formation via Michael addition of thiols to α,β -unsaturated ketones under solvent-free conditions


Samiran Bhattacharjee, James A. Anderson

Journal of Molecular Catalysis A: Chemical 249 (2006) 103

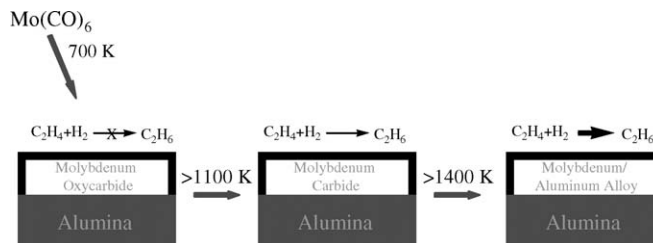
Comparison of the epoxidation of cyclohexene, dicyclopentadiene and 1,5-cyclooctadiene over LDH hosted Fe and Mn sulfonato-salen complexes



Feng Gao, Yilin Wang, W.T. Tysoe

Journal of Molecular Catalysis A: Chemical 249 (2006) 111

Ethylene hydrogenation on $\text{Mo}(\text{CO})_6$ derived model catalysts in ultrahigh vacuum: From oxycarbide to carbide to MoAl alloy

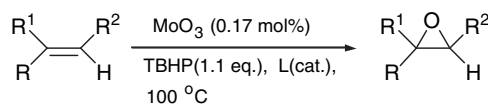


Elisabete da Palma Carreiro, Anthony J. Burke

Journal of Molecular Catalysis A: Chemical 249 (2006) 123

Catalytic epoxidation of olefins using MoO_3 and TBHP: Mechanistic considerations and the effect of amine additives on the reaction

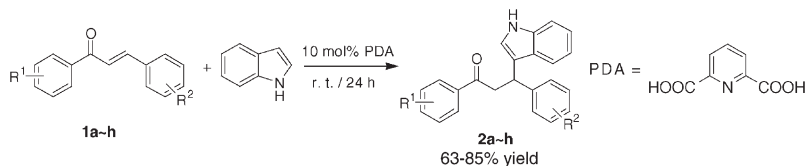
A new procedure for the catalytic epoxidation of olefins using MoO_3 as catalyst and TBHP as terminal oxidant is reported. The presence of catalytic quantities of pyridine and pyrazole accelerated the reaction.



Wei Zhou, Li-Wen Xu, Lei Yang, Pei-Qing Zhao, Chun-Gu Xia

Journal of Molecular Catalysis A: Chemical 249 (2006) 129

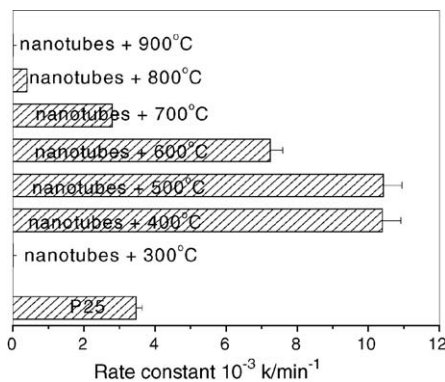
Novel brønsted acid-catalyzed Michael-type Friedel-Crafts reactions of indoles and acetalization of aldehydes



Jianguo Yu, Huogen Yu, Bei Cheng, C. Trapalis

Journal of Molecular Catalysis A: Chemical 249 (2006) 135

Effects of calcination temperature on the microstructures and photocatalytic activity of titanate nanotubes

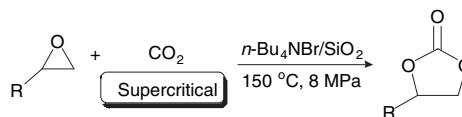


**Jin-Quan Wang, De-Lin Kong, Jian-Yu Chen,
Fei Cai, Liang-Nian He**

Journal of Molecular Catalysis A: Chemical 249
(2006) 143

Synthesis of cyclic carbonates from epoxides and carbon dioxide over silica-supported quaternary ammonium salts under supercritical conditions

Silica-supported quaternary ammonium salt proved to be a recyclable and efficient heterogeneous catalyst for the synthesis of propylene carbonate from propylene oxide and CO₂ under supercritical conditions, which requires no additional organic solvents either for the reaction or for the separation of product; the work-up procedure is straightforward and the catalyst could be reused without obvious loss of catalytic activity and selectivity. Moreover, this organic solvent-free process presented here could show much potential application in industry due to its simplicity, easy product separation from reaction medium and catalyst recycling. It could be profitably applied to the development of fix-bed continuous flow reactors, avoiding the use of solvent to isolate the products.

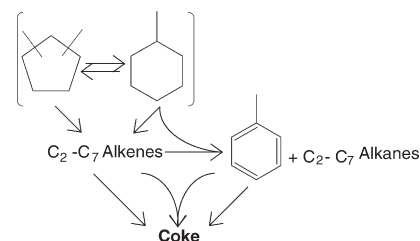


**G. Caeiro, P. Magnoux, J.M. Lopes, F. Lemos,
F. Ramôa Ribeiro**

Journal of Molecular Catalysis A: Chemical 249
(2006) 149

Kinetic modeling of the methylcyclohexane transformation over H-USY: Deactivating effect of coke and nitrogen basic compounds

In this paper, a transient pseudo-homogeneous model was developed with the objective of describing the activity, product distribution and deactivation with time on stream for the methylcyclohexane transformation over H-USY at 350°C. The reaction scheme details the reactant, cyclopentane ring isomers, alkenes, alkanes, aromatics and coke. Both the deactivating effect of coke and quinoline are described by the model. The model fits extremely well the activity, deactivation and product distribution, coke included.

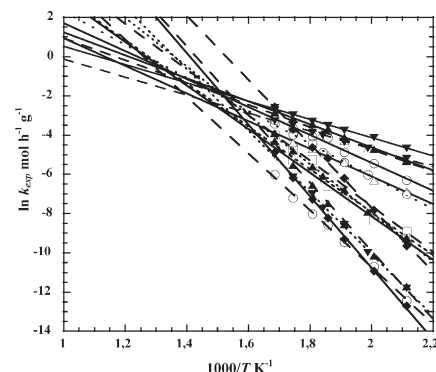


Mark A. Keane, Ragnar Larsson

Journal of Molecular Catalysis A: Chemical 249
(2006) 158

Isokinetic behaviour in gas phase catalytic haloarene hydrodehalogenation reactions: Mechanistic considerations

The experimentally determined kinetics (see figure) for the gas phase hydrodehalogenation of a range of haloarenes over Ni/SiO₂ delivers an isokinetic temperature (T_{iso}) at 658 ± 2 K which is accounted for using the Selective Energy Transfer model in terms of resonance between the out-plane C-H vibrations of substituted benzene and Ni-H vibration at high hydrogen surface coverage.

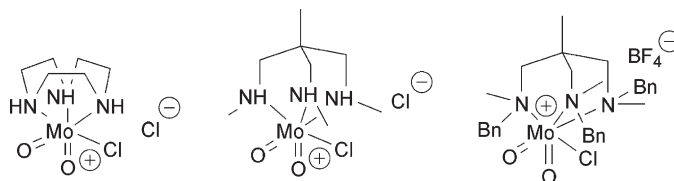


**Željko Petrovski, Anabela A. Valente,
Martyn Pillinger, Ana S. Dias, Sandra S.
Rodrigues, Carlos C. Romão, Isabel S.
Gonçalves**

Journal of Molecular Catalysis A: Chemical 249
(2006) 166

Molybdenum(VI) oxides bearing 1,4,7-triazacyclononane and 1,1,1-tris(aminomethyl)ethane ligands: Synthesis and catalytic applications

Reaction of the solvent adduct MoO₂Cl₂(solv)₂ with tridentate N-ligands based on either 1,4,7-triazacyclononane (tacn) or 1,1,1-tris(aminomethyl)ethane (tame) leads to octahedral cationic complexes, which are moderately active catalysts for the epoxidation of olefins with *t*-BuOOH. It is also shown that the tricarbonyl compounds (Me₃-tame)M(CO)₃ (M=Mo, Cr) can be used directly as catalyst precursors for olefin epoxidation since under the applied reaction conditions they undergo oxidative decarbonylation into high oxidation state oxo complexes.

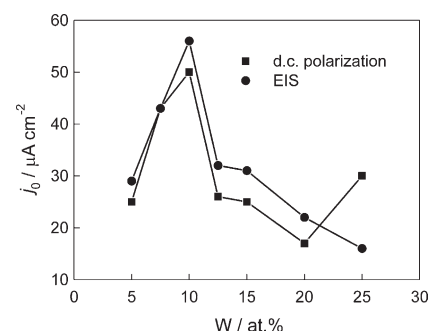


M. Metikoš-Huković, Z. Grubač, N. Radić, A. Tonejc

Journal of Molecular Catalysis A: Chemical 249 (2006) 172

Sputter deposited nanocrystalline Ni and Ni-W films as catalysts for hydrogen evolution

Nanocrystalline Ni and Ni-W alloy coatings prepared by the dc magnetron sputtering deposition method are very interesting materials due to their mechanical, catalytic and corrosion properties. The dependence of the electrocatalytic activity for the hydrogen evolution on the W content in the Ni-W catalysts is shown in the figure. The best performance demonstrates the Ni₉₀-W₁₀ alloy in accordance with the prediction based on the electronic structure.

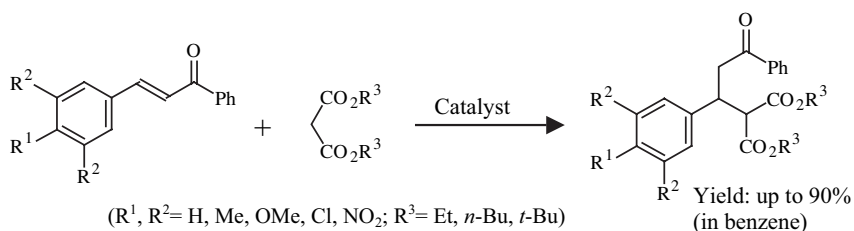


Yoshihiro Kubota, Hisanori Ikeya, Yoshihiro Sugi, Takashi Yamada, Takashi Tatsumi

Journal of Molecular Catalysis A: Chemical 249 (2006) 181

Organic-inorganic hybrid catalysts based on ordered porous structures for Michael reaction

Silicate-organic composite material (SOCM), such as MCM-41-cetyltrimethylammonium composite material, was found to be an effective base catalyst for the Michael reaction of chalcone derivative with malonic ester, whereas aminopropyl-grafted MCM-41 was less active in a non-polar solvent.

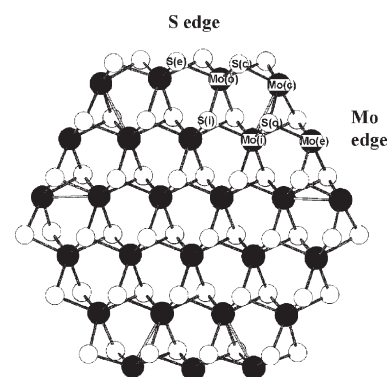


Xiao-Dong Wen, Tao Zeng, Bo-Tao Teng, Fu-Qiang Zhang, Yong-Wang Li, Jianguo Wang, Haijun Jiao

Journal of Molecular Catalysis A: Chemical 249 (2006) 191

Hydrogen adsorption on a Mo₂₇S₃₄ cluster: A density functional theory study

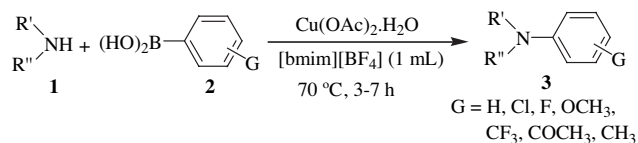
The intersection of sulfur and molybdenum edges with the formation of Mo-H and S-H bonds represents the most stable adsorption form of heterolytic hydrogen dissociation.



M. Lakshmi Kantam, B. Neelima, Ch. Venkat Reddy, V. Neeraja

Journal of Molecular Catalysis A: Chemical 249 (2006) 201

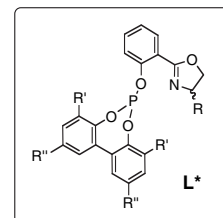
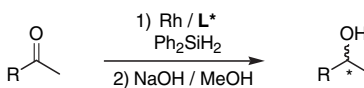
N-Arylation of imidazoles, imides, amines, amides and sulfonamides with boronic acids using a recyclable Cu(OAc)₂H₂O/[bmim][BF₄] system



Oscar Pàmies, Carmen Claver,
Montserrat Diéguez

Journal of Molecular Catalysis A: Chemical 249
(2006) 207

Phosphite–oxazoline ligands for Rh-catalyzed
asymmetric hydrosilylation of ketones

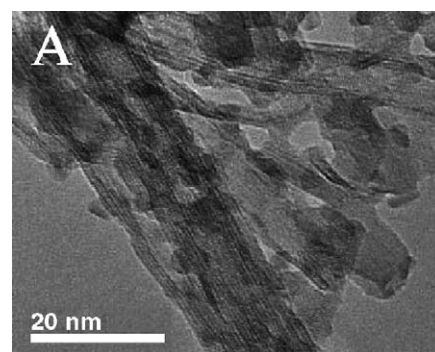


Baolin Zhu, Qi Guo, Xueliang Huang,
Shurong Wang, Shoumin Zhang, Shihua Wu,
Weiping Huang

Journal of Molecular Catalysis A: Chemical 249
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Characterization and catalytic performance of TiO₂
nanotubes-supported gold and copper particles

Gold and gold–copper supported on TiO₂ nanotubes
are synthesized by deposition–precipitation method.
The influence of preparation conditions as well as
gold content on the catalytic performance of the
modified nanotubes is investigated. After copper is
added, the modified nanotubes show better catalytic
performance.

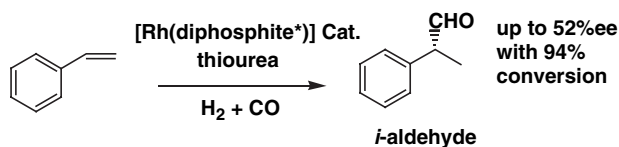


Radwan Abdallah, Jérémy A.J. Breuzard,
Michel C. Bonnet, Marc Lemaire

Journal of Molecular Catalysis A: Chemical 249
(2006) 218

Phosphite and thiourea ligand synergy for rhodium
catalyzed enantioselective hydroformylation of
styrene

New non-C₂-symmetric chiral diphosphites have been synthesized and used as ligands in the rhodium catalyzed enantioselective and regioselective hydroformylation of styrene. A synergistic effect improving both activity and enantioselectivity is observed when a chiral dithiourea is introduced as co-ligand in the Rh-diphosphite catalytic system.

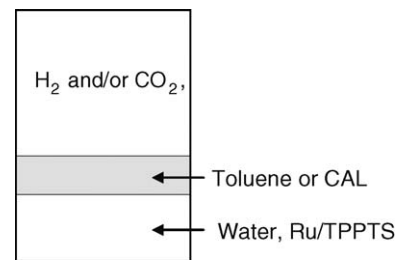


Shin-ichiro Fujita, Shuji Akihara,
Masahiko Arai

Journal of Molecular Catalysis A: Chemical 249
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Recyclability of water-soluble ruthenium–
phosphine complex catalysts in multiphase selective
hydrogenation of cinnamaldehyde using toluene and
pressurized carbon dioxide

The recycling performance of water-soluble
Ru/TPPTS complex catalysts was studied in
multiphase hydrogenation of *trans*-cinnamaldehyde
(CAL) using either toluene or carbon dioxide at low
and high pressures.



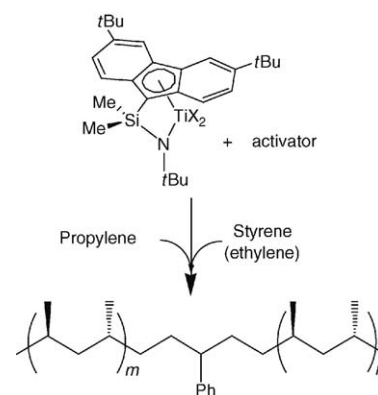
Multiphase hydrogenation

**Evgueni Kirillov, Abbas Razavi,
Jean-François Carpentier**

Journal of Molecular Catalysis A: Chemical 249 (2006) 230

Syndiotactic-enriched propylene–styrene copolymers using fluorenyl-based half-titanocene catalysts

The constrained geometry complexes $\{3,6\text{-}t\text{Bu}_2\text{C}_{13}\text{H}_6\text{SiMe}_2\text{N}^t\text{Bu}\}\text{TiX}_2$ ($\text{X}=\text{Cl}$, **1**; Me , **2**), in combination with MAO or borane activators, efficiently copolymerize propylene and styrene in the presence of small amounts of ethylene to afford styrene–propylene (PP–PS) copolymers with a syndiotactic-enriched polypropylene microstructure and randomly distributed single styrene or short polystyrene units.

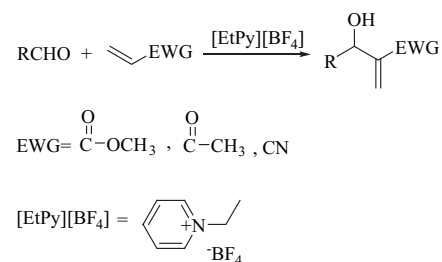


**Hang Gong, Chang-qun Cai, Nian-fa Yang,
Li-wen Yang, Jin Zhang, Qing-hua fan**

Journal of Molecular Catalysis A: Chemical 249 (2006) 236

Application of non-imidazolium-based ionic liquid in the Baylis–Hillman reactions: Rate and yield promoted

The application of non-imidazolium-based ionic liquid $[\text{EtPy}][\text{BF}_4]$ (*N*-1-ethylpyridinium tetrafluoroborate) as recyclable solvent for the Baylis–Hillman reactions is presented. Compared with the commonly used imidazolium-based ionic liquid $[\text{bmim}][\text{PF}_6]$ (1-*n*-butyl-3-methylimidazolium hexafluorophosphate) and $[\text{bdmim}][\text{PF}_6]$ (1-*n*-butyl-2,3-dimethylimidazolium hexafluorophosphate) that evidently reacts with aldehydes under basic conditions, ionic liquid $[\text{EtPy}][\text{BF}_4]$ is inert and the Baylis–Hillman reaction in $[\text{EtPy}][\text{BF}_4]$ proceeds quickly with good yields.

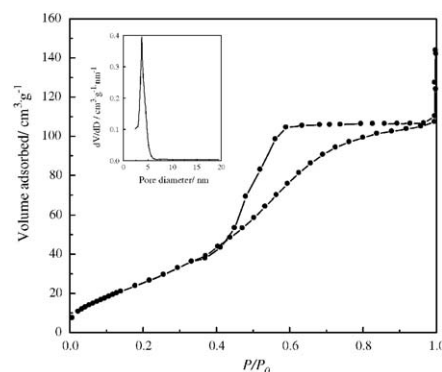


**Zhi-Qiang Zou, Ming Meng, Jin-Yong Luo,
Yu-Qing Zha, Ya-Ning Xie, Tian-Dou Hu,
Tao Liu**

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A novel mesoporous oxidation catalyst La-Co-Zr-O prepared by using nonionic and cationic surfactants as co-templates

A novel mesoporous mixed oxide catalyst La-Co-Zr-O was successfully prepared by citric acid complexation-organic template decomposition method, using *p*-octyl polyethylene glycol phenyl ether (OP) and cetyltrimethyl-ammonium bromide (CTAB) as co-templates. The sample possesses uniform mesopore diameter distribution (3.5–4.3 nm) and big specific surface area (117.6 m²/g). Its activity for CO oxidation is much better than those prepared by using single template CTAB or by co-precipitation method.



Ahmad Shaabani, Abbas Rahmati

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Silica sulfuric acid as an efficient and recoverable catalyst for the synthesis of trisubstituted imidazoles

