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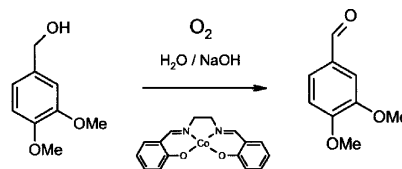
Articles

**Kaisa Kervinen, Heikki Korpi,
Markku Leskelä, Timo Repo**

Journal of Molecular Catalysis A: Chemical
203 (2003) 9

Oxidation of veratryl alcohol by molecular oxygen in aqueous solution catalyzed by cobalt salen-type complexes: the effect of reaction conditions

Cobalt salen-type complexes catalyze the selective oxidation of veratryl alcohol to veratraldehyde by molecular oxygen in basic aqueous solution. This reaction is strongly affected by the chosen reaction conditions, such as pH, temperature, pressure and the catalyst:substrate ratio.

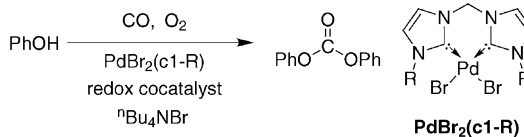


**Ken-ichi Okuyama, Jun-ichi Sugiyama,
Ritsuko Nagahata, Michihiko Asai,
Mitsuru Ueda, Kazuhiko Takeuchi**

Journal of Molecular Catalysis A: Chemical
203 (2003) 21

Oxidative carbonylation of phenol to diphenyl carbonate catalyzed by Pd–carbene complexes

Pd–carbene complexes with bis(heterocyclic carbene) ligands PdBr₂(c1-R) were found to be efficient catalysts for oxidative carbonylation of phenol to diphenyl carbonate, where catalysts were composed of Pd complex/Ce(TMHD)₄ (TMHD: 2,2,6,6-tetramethyl-3,5-heptanedionate)/hydroquinone/ⁿBu₄NBr/molecular sieve 3 Å. The Pd–carbene complex systems showed high activity compared to a conventional catalytic system.

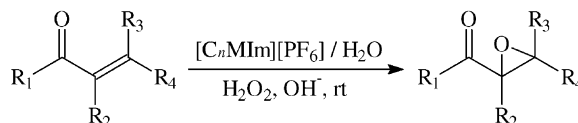


**Bo Wang, Yu-Ru Kang, Li-Ming Yang,
Ji-Shuan Suo**

Journal of Molecular Catalysis A: Chemical
203 (2003) 29

Epoxidation of α,β -unsaturated carbonyl compounds in ionic liquid/water biphasic system under mild conditions

Epoxidation reactions of α,β -unsaturated carbonyl compounds were conducted in ionic liquid/water biphasic systems using hydrogen peroxide as an oxidant at room temperature. In the epoxidation of mesityl oxide, 100% conversion and 98% selectivity were achieved under mild conditions. The mass transfer model for the epoxidation of α,β -unsaturated carbonyl compounds in the [C₄MIm][PF₆]/water biphasic system has also been proposed.

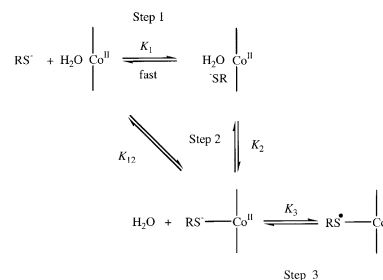


**Eduard M. Tyapochkin,
Evgenii I. Kozliak**

Journal of Molecular Catalysis A: Chemical
203 (2003) 37

Interactions of cobalt tetrasulfophthalocyanine with alkyl xanthogenates: evidence for hydrophobic effects in the Merox process

Anaerobic complexation of cobalt tetrasulfophthalocyanine (CoTSPc) with alkyl xanthogenates [ROC(S)S⁻] has been studied by UV-Vis spectroscopy to obtain evidence for the substrate-catalyst hydrophobic interactions in the Merox process (auto-oxidation of thiols in the presence of CoTSPc in aqueous solutions). In aqueous solutions but not in DMF, both binding and kinetic constants depend on the size of the substrate alkyl group.

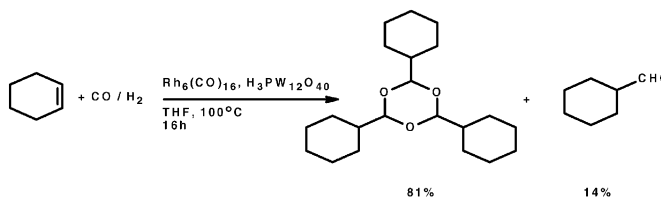


Bassam El Ali

Journal of Molecular Catalysis A: Chemical
203 (2003) 53

Rh₆(CO)₁₆-H₃PW₁₂O₄₀-catalyzed one pot hydroformylation-cyclotrimerization of cyclohexene and cyclopentene into 2,4,6-trisubstituted-1,3,5-trioxanes

A new one pot reaction of hydroformylation-cyclotrimerization of cyclopentene **1a** and cyclohexene **1b** was selectively catalyzed by Rh₆(CO)₁₆ and H₃PW₁₂O₄₀·xH₂O (HPA-W₁₂) in THF as a solvent at 600 psi (CO/H₂ = 1/1) to give 2,4,6-trisubstituted-1,3,5-trioxanes **3a** and **3b** as new and major products along with the corresponding aldehyde **2**. The effects of the type of the catalyst, co-catalyst and the type of solvent have been studied.

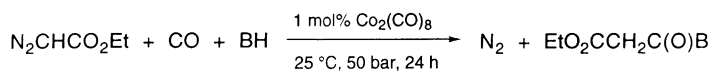


Robert Tuba, Ferenc Ungváry

Journal of Molecular Catalysis A: Chemical
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Octacarbonyl dicobalt-catalyzed selective transformation of ethyl diazoacetate into organic products containing the ethoxycarbonyl carbene building block

In the presence of 1 mol% octacarbonyl dicobalt ethyl diazoacetate can be transformed at room temperature and carbon monoxide pressure selectively into diethyl 2-diazo-3-oxoglutarate or in the presence of an alcohol (methanol, ethanol, *tert*-butanol), phenol or diethylamine into the corresponding malonic acid derivatives in high yields. Ethoxycarbonylcarbene-bridged dicobalt carbonyl complexes [μ₂-(ethoxycarbonyl(methylene))-μ₂-(carbonyl)-bis(tricarbonyl-cobalt) (Co-Co)] and [di-μ₂-(ethoxycarbonyl(methylene))-bis(tricarbonyl-cobalt) (Co-Co)] proved to be intermediates in the catalytic reactions.



(B = N₂CCO₂Et, MeO, EtO, ^tBuO, PhO, Et₂N)

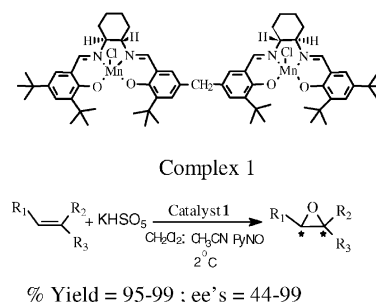
up to 96% yield

**Rukhsana Ilyas Kureshy,
Noor-ul Hasan Khan,
Sayed Hasan Razi Abdi, Irshad Ahmed,
Surendra Singh, Raksh Vir Jasra**

Journal of Molecular Catalysis A: Chemical
203 (2003) 69

Enantioselective epoxidation of non-functionalised alkenes catalysed by dimeric homochiral Mn(III) Salen complex using oxone as oxidant

Enantioselective epoxidation of non-functionalised alkenes using dimeric homochiral Mn(III) Salen complex in presence of PyN-O using KHSO₅ gave excellent epoxide yield except in indene with high chiral induction in case of nitro and cyano chromene and the catalyst could be reused up to three cycles.

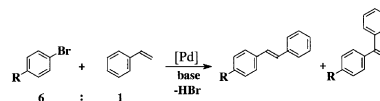


**Alexander F. Schmidt,
Vladimir V. Smirnov**

Journal of Molecular Catalysis A: Chemical
203 (2003) 75

Simple method for enhancement of the ligand-free palladium catalyst activity in the Heck reaction with non-activated bromoarenes

Simple catalytic system is reported capable of catalyzing effectively the reaction of bromoarenes with styrene in the air in the absence of any ligands. Quantitative yield of the product was achieved by the use of 0.04–1.6 mol% PdCl₂, 18% HCOONa, 112% AcONa and six-fold excess of bromoarene (with respect to styrene) in DMF after 10 min at 140° or after 180 min at 100°.



Maw-Ling Wang, Yao-Hsuan Tseng

Journal of Molecular Catalysis A: Chemical
203 (2003) 79

Phase transfer catalytic reaction of *n*-bromobutane and sodium sulfide in a two-phase solution and its kinetics

Synthesis of di-*n*-butyl sulfide (RSR; R: C₄H₉) from the reaction between sodium sulfide (Na₂S) and *n*-bromobutane (1-C₄H₉Br) in an organic solvent/alkaline solution two-phase medium under phase transfer catalysis (PTC) conditions are described.

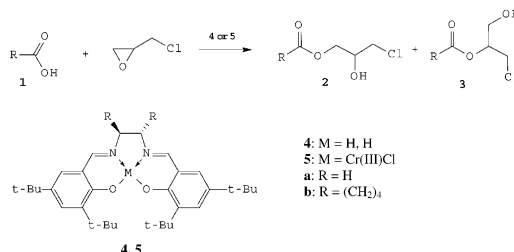


**Agnieszka Bukowska, Wiktor Bukowski,
Jarosław Noworól**

Journal of Molecular Catalysis A: Chemical
203 (2003) 95

A study on the addition of some carboxylic acids to epichlorohydrin in the presence of salen chromium(III) complexes

The effect of salen ligands on the catalytic activity and regioselectivity of chromium(III) ions in the addition reaction of aliphatic carboxylic acids to epichlorohydrin was studied. It was found that coordination of chromium(III) ions by tetradentate Schiff's bases decreased their catalytic activity in comparison to chromium(III) acetate. Slightly worse regioselectivity was also detected.

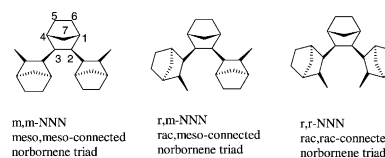


Ralf Alexander Wendt, Gerhard Fink

Journal of Molecular Catalysis A: Chemical
203 (2003) 101

Ethene–norbornene copolymerizations using two different homogeneous metallocene catalyst systems and investigations of the copolymer microstructure

Ethene–norbornene copolymers generated with the metallocene *i*Pr[(3-*i*Pr-Cp)Ind]ZrCl₂ contain norbornene microblocks with a maximum length of two norbornene units, whereas in copolymers generated with the metallocene *rac*-*i*Pr[Ind]₂ZrCl₂ norbornene microblocks with a length of three norbornene units (triblocks) have been detected. The amount of norbornene triblocks as well as the stereochemical connection of the triblocks depends on the monomer concentration and the polymerization temperature.

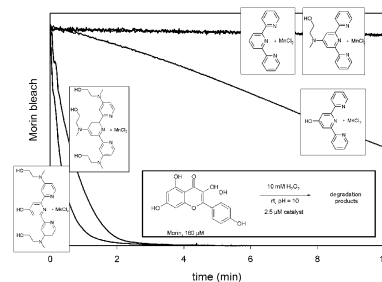


**Torsten Wieprecht, Juntao Xia,
Uwe Heinz, Josef Dannacher,
Gunther Schlingloff**

Journal of Molecular Catalysis A: Chemical
203 (2003) 113

Novel terpyridine-manganese(II) complexes and their potential to activate hydrogen peroxide

Novel manganese(II) complexes with substituted terpyridine (terpy) ligands are described as catalyst for oxidation processes with hydrogen peroxide. Introduction of π -donor substituents in the 4-positions of the pyridine rings resulted in an enhanced catalytic activity compared to the unsubstituted complex on Morin in alkaline aqueous solution. Complex formation, pH and substrate dependence of the catalysts have been investigated.

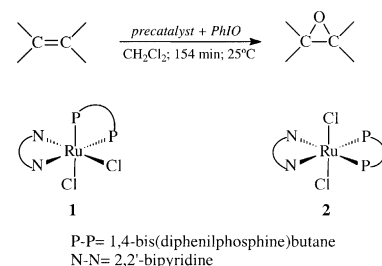


**André L. Bogado, Roberto F. de Souza,
Ulf Schuchardt, Alzir A. Batista**

Journal of Molecular Catalysis A: Chemical
203 (2003) 129

On the kinetics of epoxidation of olefins by *cis* and *trans*-[RuCl₂(dppb)(2,2'-bipy)] complexes

The Michaelis–Menten plots and their corresponding Lineweaver–Burk plots, have shown to be a convenient method for the kinetic study of this catalytic reaction, in order to obtain the corresponding V_{\max} and K_M parameters.

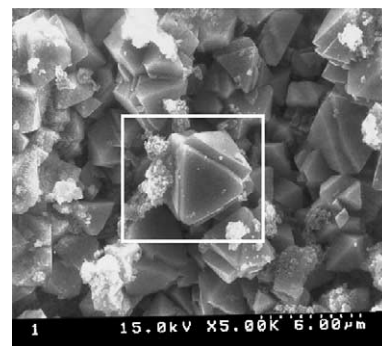


**Man Seok Han, Byung Gwon Lee,
Byoung Sung Ahn, Hoon Sik Kim,
Dong Ju Moon, Suk In Hong**

Journal of Molecular Catalysis A: Chemical
203 (2003) 137

The role of copper chloride hydroxides in the oxidative carbonylation of methanol for dimethyl carbonate synthesis

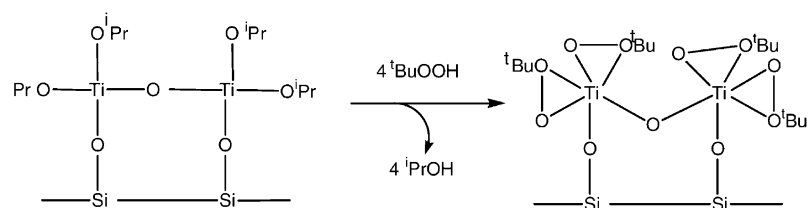
This is the SEM image of CuCl₂/NaOH/AC catalyst with molar ratio of OH/Cu = 1.0. An interesting crystal structure was observed and confirmed to be *paratacamite* (rhombohedral) by using various surface analyzers. It has shown a higher activity to DMC synthesis than CuCl₂/AC. This kind of crystal habit was not observed at all in the SEM image of CuCl₂/AC catalyst free of NaOH.



**Soumen Sensarma, Abdillahi Omar Bouh,
Susannah L. Scott, Howard Alper**

Journal of Molecular Catalysis A: Chemical
203 (2003) 145

Olefin epoxidation catalyzed by an air stable-supported titanium catalyst

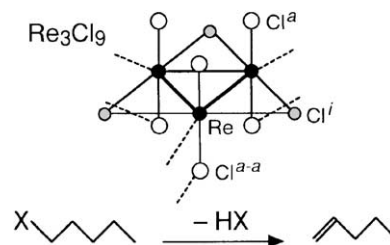


**Satoshi Kamiguchi, Masaki Watanabe,
Kunihiko Kondo, Mitsuo Kodomari,
Teiji Chihara**

Journal of Molecular Catalysis A: Chemical
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Catalytic dehydrohalogenation of alkyl halides by Nb, Mo, Ta, and W halide clusters with an octahedral metal framework and by a Re chloride cluster with a triangular metal framework

Molecular halide clusters of Nb, Mo, Ta, and W developed catalytic activity for dehydrohalogenation of halogenated pentanes when treated in helium or hydrogen stream at 300 °C. Solid state Re_3Cl_9 also developed the activity in a stream of helium. When Re_3Cl_9 was treated in a stream of hydrogen, it changed to metallic Re, which catalyzed both dehydrohalogenation and hydrodehalogenation concurrently.

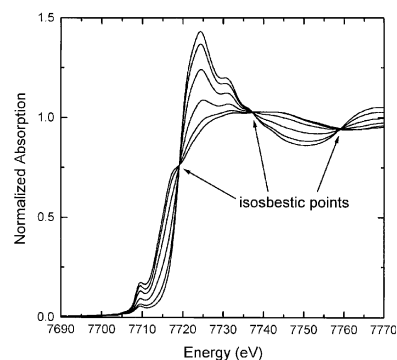


**Jyh-Fu Lee, An-Chyi Wei,
Kuei-Jung Chao**

Journal of Molecular Catalysis A: Chemical
203 (2003) 165

In situ X-ray absorption spectroscopic study on the reducibility of cobalt-containing aluminophosphate molecular sieves

Transition in the features of real-time X-ray absorption spectra (XAS) reflects the change of electronic and atomic structures of cobalt species during the reduction.

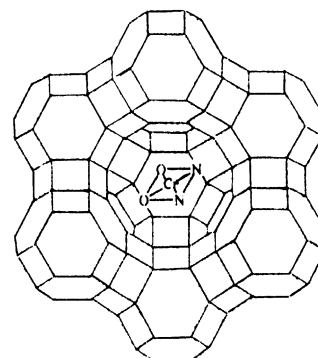


**Pratap Kumar Saha, Sandip Saha,
Subratanath Koner**

Journal of Molecular Catalysis A: Chemical
203 (2003) 173

Chromotropism of Cr(salen) moiety in zeolite matrix: synthesis, characterization and catalytic activity study of Cr(salen)-NaY hybrid catalyst

On immobilization in zeolite matrix, the $[\text{Cr}(\text{salen})]^+$ complex moiety showed a remarkable color change from yellow to light grey. An excellent catalytic performance of the newly prepared hybrid catalysts was observed in epoxidation reaction of norbornene and styrene.

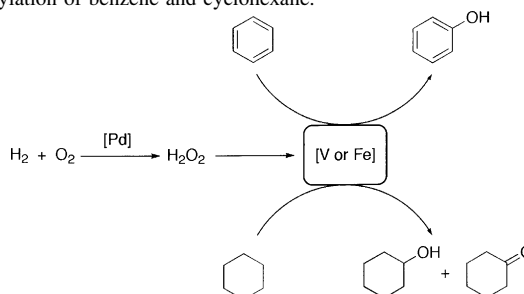


**Joseph E. Remias, Thomas A. Pavlosky,
Ayusman Sen**

Journal of Molecular Catalysis A: Chemical
203 (2003) 179

Catalytic hydroxylation of benzene and cyclohexane using in situ generated hydrogen peroxide: new mechanistic insights and comparison with hydrogen peroxide added directly

Metallic palladium-catalyzed *in situ* hydrogen peroxide generation from dihydrogen and dioxygen is coupled with a vanadium or iron catalyst that utilizes the hydrogen peroxide for the hydroxylation of benzene and cyclohexane.

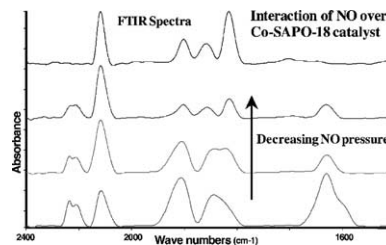


**Chris Kladis, Suresh K. Bhargava,
Deepak B. Akolekar**

Journal of Molecular Catalysis A: Chemical
203 (2003) 193

Interaction of probe molecules with active sites on cobalt, copper and zinc-exchanged SAPO-18 solid acid catalysts

In situ FTIR of NO/CO studies were conducted on the in-house prepared and well characterized Co-, Cu- and Zn-exchanged SAPO-18 solid acid catalysts. NO adsorption leads to the formation of adsorbed N_2O , chemisorbed NO_2 and nitrite, mononitrosyl and dinitrosyl complexes. CO adsorption leads to formation of physisorbed CO_2 , cationic Lewis acid carbonyl moieties and transition metal carbonyl complexes.

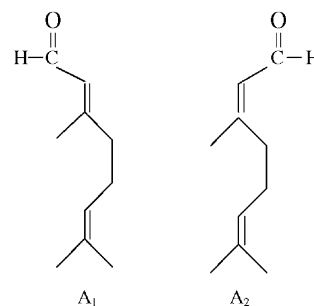


P. Reyes, H. Rojas, J.L.G. Fierro

Journal of Molecular Catalysis A: Chemical
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Effect of Fe/Ir ratio on the surface and catalytic properties in citral hydrogenation on Fe-Ir/TiO₂ catalysts

The selective hydrogenation in liquid phase of citral on Ir/TiO₂ and Fe-Ir/TiO₂ catalysts have been studied. The addition of Fe³⁺ species lead to an increase in the polarization of the C=O bond producing an enhancement in the reaction rate. Similar effect is displayed by Ir/TiO₂ catalysts reduced at high temperature due to surface decoration of the metallic crystals by TiO_x moieties. Geraniol and nerol are the most important obtained products.



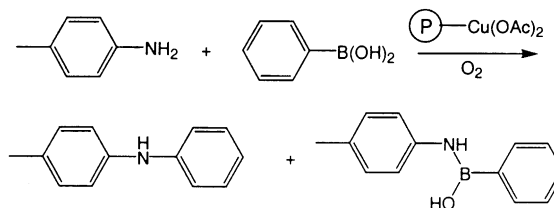
A₁: Citral E. A₂: Citral Z

**A. Biffis, F. Filippi, G. Palma, S. Lora,
C. Maccà, B. Corain**

Journal of Molecular Catalysis A: Chemical
203 (2003) 213

Metallation of functional resins with copper acetate: control of metal speciation and catalytic activity in C–N coupling reactions

Tailor-made gel-type resins bearing acid groups were reacted with Cu(OAc)₂ under various experimental conditions. In this way, different kinds of resin-supported copper(II) species can be obtained, some of which exhibit promising catalytic activity in C–N coupling reactions.

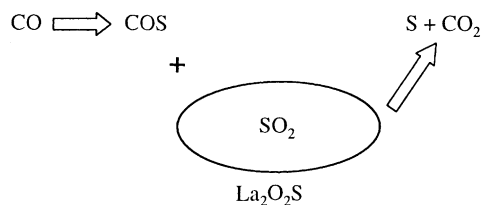


Ngai T. Lau, Ming Fang, Chak K. Chan

Journal of Molecular Catalysis A: Chemical
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Reduction of SO₂ by CO and COS over La₂O₂S—a mechanistic study

The redox route, in which anion vacancies in the catalyst are created by reduction and reduce SO₂ to sulfur, is not the main reaction path for the catalytic reduction of SO₂ by CO and COS over La₂O₂S. The TPR/MS and feed-perturbation experiments indicate that the reaction probably proceeds through the COS intermediate, which reacts with pools of strongly adsorbed SO₂ to produce sulfur.

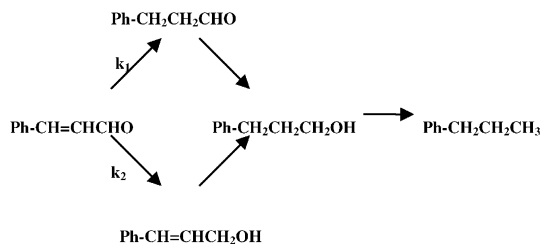


A. Hammoudeh, S. Mahmoud

Journal of Molecular Catalysis A: Chemical
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Selective hydrogenation of cinnamaldehyde over Pd/SiO₂ catalysts: selectivity promotion by alloyed Sn

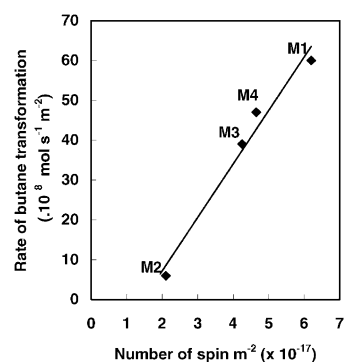
Sn was found to enhance the catalytic selectivity of Pd/SiO₂ in the liquid-phase hydrogenation of cinnamaldehyde by increasing the rate constant ratio (k_2/k_1) of the hydrogenation route to cinnamyl alcohol to that producing phenylpropanal. This promotion effect is attributed to both geometric and electronic effects of alloying Pd with Sn.

**Ioan-Cezar Marcu, Ioan Sandulescu, Jean-Marc M. Millet**

Journal of Molecular Catalysis A: Chemical
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Effects of the method of preparing titanium pyrophosphate catalyst on the structure and catalytic activity in oxidative dehydrogenation of *n*-butane

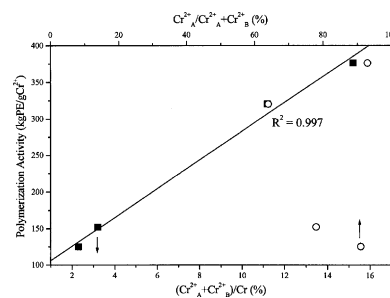
The catalytic properties in the ODH of *n*-butane of titanium pyrophosphate (TiP₂O₇) have been related to their redox and acid-base properties. A linear relationship was observed between the reduction extent by *n*-butane measured by ESR and the rate of *n*-butane conversion showing that the activity depends on the titanium ability to undergo oxido-reduction. This confirmed previous results showing that the limiting step was the re-oxidation of the catalyst.

**A.B. Gaspar, J.L.F. Brito, L.C. Dieguez**

Journal of Molecular Catalysis A: Chemical
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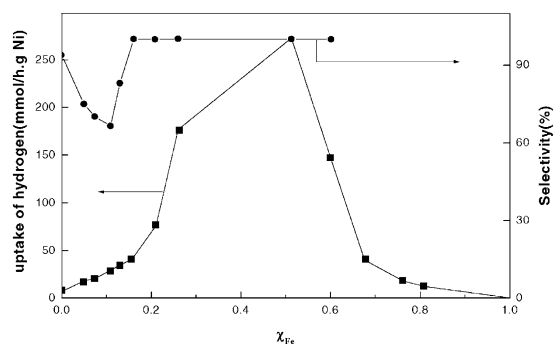
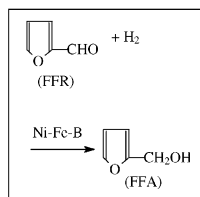
Characterization of chromium species in catalysts for dehydrogenation and polymerization

Chromium catalysts, prepared with different chromium contents, supports and precursor compounds, were characterized by O₂ and CO chemisorption, in order to quantify the Cr³⁺ and Cr²⁺ sites, respectively. The distribution of chromium species, which depends on the preparation parameters, was related to the catalytic activity in the dehydrogenation and polymerization reactions.

**Hexing Li, Hongshan Luo, Li Zhuang, Weilin Dai, Minghua Qiao**

Journal of Molecular Catalysis A: Chemical
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Liquid phase hydrogenation of furfural to furfuryl alcohol over the Fe-promoted Ni-B amorphous alloy catalysts

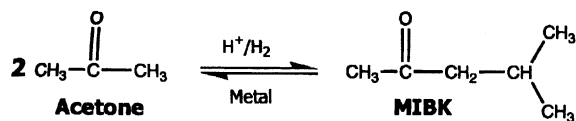


**Ricardo Morales, Luis Melo,
Joaquín Brito, Aura Llanos,
Delfín Moronta, Luis Albornoz,
Eloy Rodríguez**

Journal of Molecular Catalysis A: Chemical
203 (2003) 277

Acetone transformation over PtSn/H[Al]-
ZSM5 catalysts

The following reaction was studied,



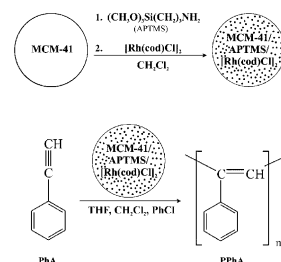
The results obtained show a sensitive variation in the catalytic properties as X_{Sn} is varied in the series of PtSn/H[Al]ZSM5 catalysts prepared (assessed by XPS, EPR and TEM); these changes are attributed to the presence of the electronic and geometric type.

**Hynek Balcar, Jiří Čejka, Jan Sedláček,
Jan Svoboda, Jiří Zedník, Zdeněk Bastl,
Vladimír Bosáček, Jiří Vohlídal**

Journal of Molecular Catalysis A: Chemical
203 (2003) 287

[Rh(cod)Cl]₂ complex immobilized on meso-
porous molecular sieves MCM-41-a new
hybrid catalyst for polymerization of phenyl-
acetylene

New hybrid catalyst affording polymeriza-
tion of phenylacetylene into high-molecu-
lar-weight ($M_w = 180\,000$) high-*cis*-polyphenyl-
acetylene (PPhA) was prepared via immobi-
lization of [Rh(cod)Cl]₂ (cod = η^4 -
cycloocta-1,5-diene) on MCM-41 modified
by 3-aminopropyltrimethoxysilane. In com-
parison with related homogeneous catalysis,
hybrid catalyst was found to provide compar-
able or even higher PPhA yields, higher
molecular weight of PPhA and reduced
amounts of oligomeric by-products.

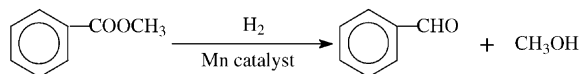


**Aimin Chen, Hualong Xu, Yinghong Yue,
Weiming Hua, Wei Shen, Zi Gao**

Journal of Molecular Catalysis A: Chemical
203 (2003) 299

Support effect in hydrogenation of methyl
benzoate over supported manganese oxide
catalysts

Benzaldehyde can be obtained via hydrogenation of methyl benzoate on supported manganese oxide catalysts with high yield, in particular, on Mn/ γ -Al₂O₃ catalyst. The support effect of MgO, γ -Al₂O₃, TiO₂, ZrO₂, SiO₂ and SiO₂-Al₂O₃ in the catalytic reaction has been studied.



Dianyu Chen, Zhigang Xue, Zhixing Su

Journal of Molecular Catalysis A: Chemical
203 (2003) 307

A new catalyst of 12-molybdophosphoric
acid for cationic polymerization of styrene:
activity and mechanism studies

12-Molybdophosphoric acid was introduced
in this paper into the polymerization of sty-
rene. High catalysis efficiency was found that
84% of monomer was reacted in less than 20
minutes. After a serial of characterization, the
reaction mechanism was put forward as elec-
tron coordination-cationic polymerization
theory, and the aimed catalyst was played
as both oxidation agent, initiator and operate
anion of the growing cationic center.

