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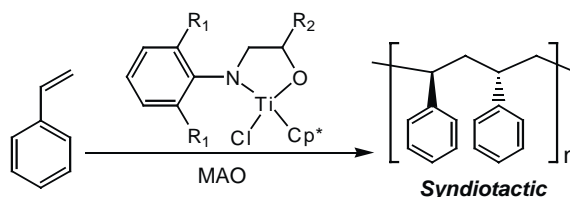
Articles

Jie Chen, Yue-Sheng Li, Ji-Qian Wu, Ning-Hai Hu

Journal of Molecular Catalysis A: Chemical 232 (2005) 1

Synthesis and styrene polymerization behavior of new titanium complexes $\text{Cp}^*\text{TiCl}(\text{OCHRCH}_2\text{NAr})$

A series of new titanium complexes $\text{Cp}^*\text{TiCl}(\text{OCHRCH}_2\text{NAr})$ has been synthesized and characterized, and is shown to be high active catalysts for the syndiospecific polymerization of styrene.

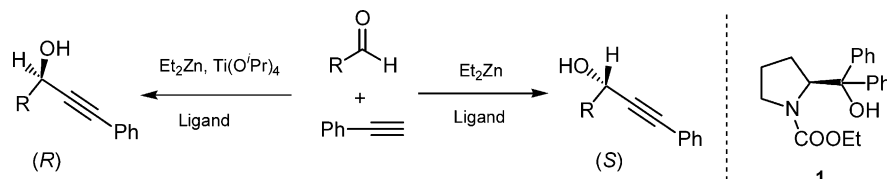


Jincheng Mao, Boshun Wan, Fan Wu, Rongliang Wang, Shiwei Lu

Journal of Molecular Catalysis A: Chemical 232 (2005) 9

Reversal of stereochemistry by adding $\text{Ti}(\text{O}^i\text{Pr})_4$ in the enantioselective phenylacetylene addition to aldehydes using 1-prolinol-backbone ligand

The readily synthesized chiral ligand **1** in combination with $\text{Ti}(\text{O}^i\text{Pr})_4$ provided the products with opposite absolute configuration in significant enantiomeric excesses and high yields. The ratio of $\text{Ti}(\text{O}^i\text{Pr})_4$ to the ligand had great influence on the enantiomeric excess of the product.

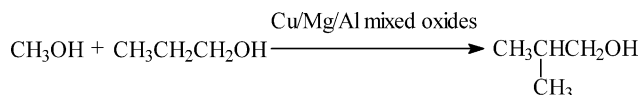


Carlo Carlini, Mario Marchionna, Marilena NovIELLO, Anna Maria Raspolli Galletti, Glauco Sbrana, Francesco Basile, Angelo Vaccari

Journal of Molecular Catalysis A: Chemical 232 (2005) 13

Guerbet condensation of methanol with *n*-propanol to isobutyl alcohol over heterogeneous bifunctional catalysts based on Mg–Al mixed oxides partially substituted by different metal components

The synthesis of isobutyl alcohol, via the Guerbet condensation of methanol with *n*-propanol, was studied. Bifunctional heterogeneous catalysts based on dehydrogenating/hydrogenating metals (Pd, Rh, Ni or Cu) and basic Mg/Al mixed oxides, obtained from hydrotalcite-type (HT) precursors, were investigated. Co-precipitated systems based on Cu/Mg/Al mixed oxides revealed the best performances, in terms of activity and selectivity.

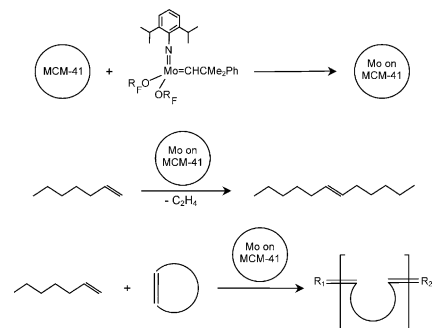


Hynek Balcar, Naděžda Žilková, Jan Sedláček, Jiří Zedník

Journal of Molecular Catalysis A: Chemical 232 (2005) 53

MCM-41 anchored Schrock catalyst $\text{Mo}(\text{=CHCMe}_2\text{Ph})(\text{=N-2,6-}i\text{-Pr}_2\text{C}_6\text{H}_3)[\text{OCMe}(\text{CF}_3)_2]_2$ -activity in 1-heptene metathesis and cross-metathesis reactions

Hybrid catalyst for olefin metathesis was prepared by anchoring Schrock carbene complex on mesoporous molecular sieve MCM-41.



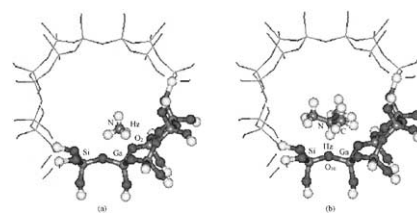
Nan Jiang, Shuping Yuan, Jianguo Wang, Zhangfeng Qin, Haijun Jiao, Yong-Wang Li

Journal of Molecular Catalysis A: Chemical 232 (2005) 59

An ONIOM study of amines adsorption in H-[Ga]MOR

The adsorption of amines (NH_3 , MeNH_2 , Me_2NH and Me_3N) in two stable bridging oxygen sites (O_{10}H and O_2H) in H-[Ga]MOR clusters is investigated by using the ONIOM2 method. All amines are protonated and the formed $[\text{HNR}_3]^+$ are stabilized by the H-bonds between the negatively charged zeolite oxygen atoms and the hydrogen atoms of the NH and CH bonds in the adsorbates. On the basis of the calculated adsorption energies, it is concluded that the relative basicity of amines follows the order of $\text{Me}_2\text{NH} > \text{Me}_3\text{N} > \text{MeNH}_2 > \text{NH}_3$. Due to the effect of introduced methyl groups and their different basicity and structures, NH_3 prefers to adsorb at the O_2H Brønsted site (Fig. a), while Me_2NH and Me_3N prefer to adsorb at the O_{10}H site (Fig. b), and

MeNH_2 can be in equilibrium between O_2H and O_{10}H .

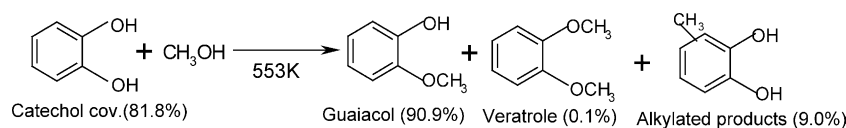


Zaihui Fu, Yan Yu, Dulin Yin, Youzhi Xu, Huiping Liu, Huiying Liao, Qiong Xu, Fuqiang Tan, Jing Wang

Journal of Molecular Catalysis A: Chemical 232 (2005) 69

Vapor-phase highly selective *O*-methylation of catechol with methanol over ZnCl_2 modified $\gamma\text{-Al}_2\text{O}_3$ catalysts

It is firstly discovered that ZnCl_2 modified $\gamma\text{-Al}_2\text{O}_3$ ($\text{ZnCl}_2/\gamma\text{-Al}_2\text{O}_3$) solid Lewis acid catalyst, which is prepared by solid-state reaction, is very active and extremely selective for the preparation of guaiacol by the vapor phase *O*-methylation of catechol with methanol in a fixed-bed reactor at 553K.

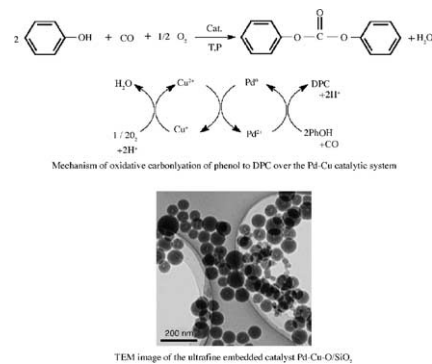


Wei Xue, Jingchang Zhang, Yanji Wang, Qian Zhao, Xinqiang Zhao

Journal of Molecular Catalysis A: Chemical 232 (2005) 77

Effect of promoter copper on the oxidative carbonylation of phenol over the ultrafine embedded catalyst Pd-Cu-O/SiO₂

Effect of promoter copper on the oxidative carbonylation of phenol to diphenyl carbonate (DPC) over the ultrafine embedded catalyst PdCuO/SiO₂ was studied. The promoter copper can be divided into the heterogeneous Cu(II) contained in the catalyst and the homogeneous Cu²⁺ charged into the reactor directly. They influence the activity of the catalyst through different routes.



TEM image of the ultrafine embedded catalyst Pd-Cu-O/SiO₂.

Praveen K. Tandon, Sumita Sahgal, Alok K. SinghGayatri, Manisha Purwar

Journal of Molecular Catalysis A: Chemical 232 (2005) 83

Oxidation of ketones by ceric perchlorate catalysed by iridium(III)

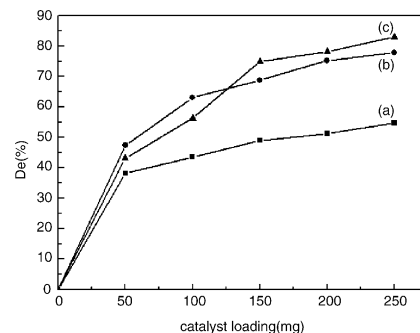
IrCl_3 , a sluggish catalyst in alkaline media, surpasses catalytic efficiency of osmium and ruthenium in aqueous perchloric acid medium in the oxidation of aliphatic ketones by ceric perchlorate. Following rate law explains all findings $-\text{dCe(IV)}/\text{dt} = 2kK_1K_2\text{Ce}^{\text{IV}}\text{SIr}^{\text{III}}\text{H}^+ + K_1K_2\text{Ce}^{\text{IV}}\text{S}$

Xinshu Niu, Honghua Li, Guoguang Liu

Journal of Molecular Catalysis A: Chemical 232 (2005) 89

Preparation, characterization and photocatalytic properties of REFeO_3 (RE = Sm, Eu, Gd)

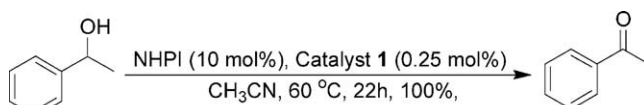
Nanometer materials of rare earth mixed oxides REFeO_3 (RE=Sm, Eu, Gd) with the structure of perovskite-type were synthesized by the sol-gel method in the citric acid system and characterized by X-ray diffractometer and TEM. These mixed oxides showed high photocatalytic activities in the degradation of various water-soluble dyes.



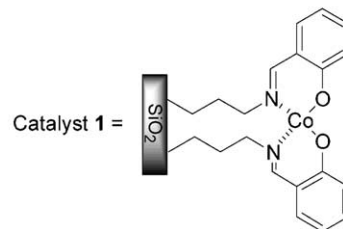
Fatemeh Rajabi, Babak Karimi

Journal of Molecular Catalysis A: Chemical 232 (2005) 95

Efficient aerobic oxidation of alcohols using a novel combination *N*-hydroxy phthalimide (NHPI) and a recyclable heterogeneous cobalt complex



The catalyst can be recovered 5 times

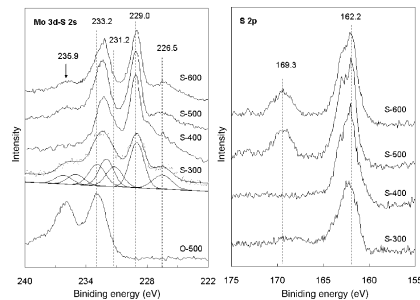


Xueqin Wang, Umit S. Ozkan

Journal of Molecular Catalysis A: Chemical 232 (2005) 101

Effect of pre-treatment conditions on the performance of sulfided Ni-Mo/ γ - Al_2O_3 catalysts for hydrogenation of linear aldehydes

Both of sulfidation and post-sulfidation degassing temperatures can be effectively used to manipulate the surface density of anion vacancy, hydroxyl, and sulfhydryl sites over sulfided Ni-Mo/ Al_2O_3 catalysts. Sulfidation temperatures in excess of 500°C , lead to the formation of a sulfate phase.

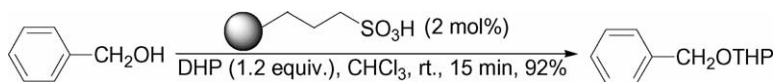


Babak Karimi, Maryam Khalkhali

Journal of Molecular Catalysis A: Chemical 232 (2005) 113

Solid silica-based sulfonic acid as an efficient and recoverable interphase catalyst for selective tetrahydropyranlation of alcohols and phenols

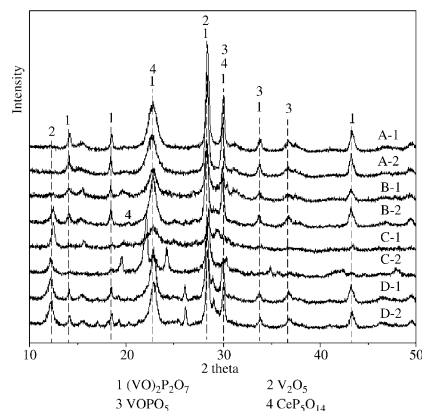
Various types of alcohols and phenols are converted to the corresponding tetrahydropyranyl (THP) ether using a catalytic amount of solid silica-based sulfonic acid. The catalyst shows high thermal stability (up to 300°C) and can be recovered and reused for at least eight reaction cycles without loss of reactivity.

**Ling Zeng, Huachang Jiang, Junfeng Niu**

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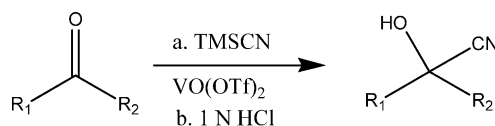
The study of L-VPO catalysts prepared by microwave methods

The L-VPO catalyst with Ce and La prepared by microwave method, showed the best activity with the yield and selectivity of acrylic acid for partial oxidation of propane.

**Surya K. De, Richard A. Gibbs**

Journal of Molecular Catalysis A: Chemical 232 (2005) 123

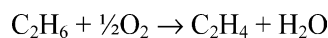
Vanadyl triflate as an efficient and recyclable catalyst for trimethylsilyl cyanide addition to carbonyl compounds

**L. Lisi, G. Ruoppolo, M.P. Casaletto, P. Galli, M.A. Massucci, P. Patrono, F. Pinzari**

Journal of Molecular Catalysis A: Chemical 232 (2005) 127

Vanadium-metal(IV)phosphates as catalysts for the oxidative dehydrogenation of ethane

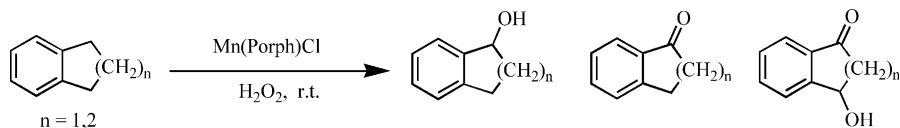
Cubic vanadium-exchanged Ti, Zr, and Sn-pyrophosphates were investigated as catalysts for the oxidative dehydrogenation of ethane. The catalytic activity is proportional to surface vanadium species, V/TiP catalyst providing the best performances due both to the good VO²⁺ exchange capacity and to the high stability. The very good ethylene selectivity, even at quite high conversion, was attributed to the great vanadium site isolation.



Susana L.H. Rebelo, Mário M.Q. Simões, M. Graça P.M.S. Neves, Artur M.S. Silva, Pietro Tagliatesta, José A.S. Cavaleiro

Journal of Molecular Catalysis A: Chemical 232 (2005) 135

Oxidation of bicyclic arenes with hydrogen peroxide catalysed by Mn(III) porphyrins

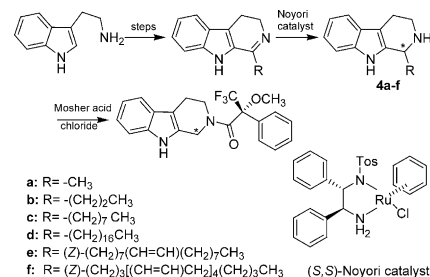


Piotr Roszkowski, Krystyna Wojtasiewicz, Andrzej Leniewski, Jan K. Maurin, Tadeusz Lis, Zbigniew Czarnocki

Journal of Molecular Catalysis A: Chemical 232 (2005) 143

Enantioselective synthesis of 1-substituted tetrahydro- β -carboline derivatives via the asymmetric transfer hydrogenation

Several 1-substituted-3,4-dihydro- β -carboline derivatives were subjected to asymmetric transfer hydrogenation catalysed by chiral ruthenium complexes to give both enantiomers of 1,2,3,4-tetrahydro- β -carbolines of high optical purity and in good yields. The absolute stereochemistry of **4c** was established on the basis of X-ray analysis of its Mosher's amide.

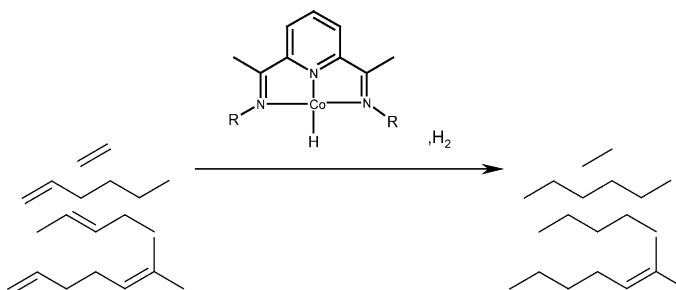


Quinten Knijnenburg, Andrew D. Horton, Harry van der Heijden, T. Martijn Kooistra, Dennis G.H. Hetterscheid, Jan M.M. Smits, Bas de Bruin, Peter H.M. Budzelaar, Anton W. Gal

Journal of Molecular Catalysis A: Chemical 232 (2005) 151

Olefin hydrogenation using diimine pyridine complexes of Co and Rh

Square-planar cobalt diimine pyridine complexes LCoR are active in the hydrogenation of monosubstituted and disubstituted olefins; sterically more hindered trisubstituted olefins do not react. Intermediate alkyl species of the hydrogenation cycle were detected. The mechanism was further investigated by EPR measurements and DFT calculations.

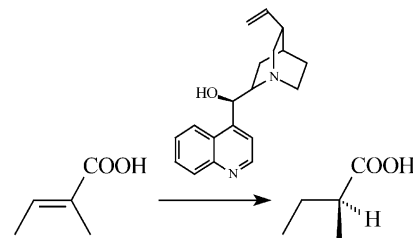


R. Bisignani, S. Franceschini, O. Piccolo, A. Vaccari

Journal of Molecular Catalysis A: Chemical 232 (2005) 161

The solvent effect in the enantioselective hydrogenation of (*E*)-2-methyl-2-butenic acid with cinchonidine doped Pd/Al₂O₃

The hydrogenation of (*E*)-2-methyl-2-butenic acid (tiglic acid), using a commercial 5wt% Pd/Al₂O₃ (Engelhard) doped with cinchonidine (CD) was investigated in depth to evidence the nature of the interaction CD:acid and the specific role of the solvent polarity on the enantiomeric excess (e.e.). A linear correlation between the dielectric constant of the solvent (ϵ) and the e.e. was observed, with a decrease in e.e. by increasing ϵ . The highest enantiomeric excess (e.e.=48%) was obtained with *n*-hexane.

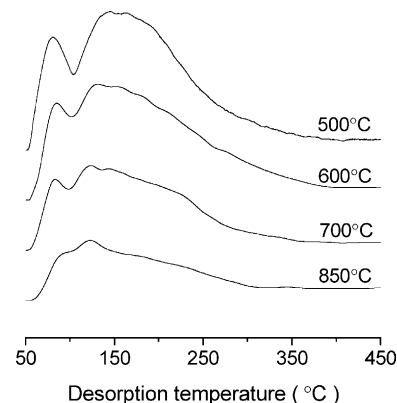


Guojie Jin, Guanzhong Lu, Yanglong Guo, Yun Guo, Junsong Wang, Weiyong Kong, Xiaohui Liu

Journal of Molecular Catalysis A: Chemical 232 (2005) 165

Effect of preparation condition on performance of Ag–MoO₃/ZrO₂ catalyst for direct epoxidation of propylene by molecular oxygen

The Ag–MoO₃/ZrO₂ catalyst for an epoxidation of propylene by molecular oxygen was prepared and characterized by N₂ adsorption, XRD, NH₃-TPD and CO₂-TPD. For the Ag–MoO₃/ZrO₂ catalyst, the lower surface area, larger pore size, modest and weaker surface acidity–basicity and suitably larger particle size of Ag are in favor of the formation of propylene oxide, which can be controlled by optimizing the preparation conditions of the ZrO₂ support and catalyst.

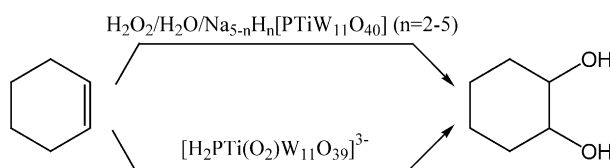


Oxana A. Kholdeeva, Tatiana A. Trubitsina, Maria N. Timofeeva, Gennadii M. Maksimov, Raisa I. Maksimovskaya, Vladimir A. Rogov

Journal of Molecular Catalysis A: Chemical 232 (2005) 173

The role of protons in cyclohexene oxidation with H₂O₂ catalysed by Ti(IV)-monosubstituted Keggin polyoxometalate

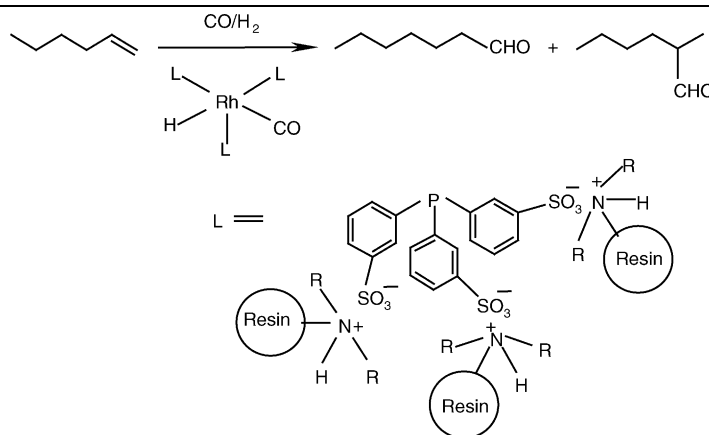
Heteropolyacid H₅PTiW₁₁O₄₀ and its acid sodium salts Na_{5-n}H_nPTiW₁₁O₄₀ (n=2–4) catalyse efficiently cyclohexene oxidation by aqueous H₂O₂ in acetonitrile via heterolytic oxygen-transfer mechanism to yield *trans*-cyclohexane-1,2-diol. The diprotonated peroxotitanium species [H₂PTi(O₂)W₁₁O₃₉]³⁻ is suggested as an active intermediate responsible for this reaction.



M.M. Diwakar, R.M. Deshpande, R.V. Chaudhari

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Hydroformylation of 1-hexene using Rh/TPPTS complex exchanged on anion exchange resin: kinetic studies



Ian D. Cunningham, Khaterah Fassihi

Journal of Molecular Catalysis A: Chemical 232 (2005) 187

Kinetics and mechanism of methyl acrylate homo- and co-polymerisation catalysed by cyclopentadienyltitanium trichloride–MAO

CpTiCl₃–MAO catalysed polymerisation and co-polymerisation of methyl acrylate and styrene occurs via insertion of an O-complexed monomer into a η³ enolate–Ti growing polymer chain. For the co-polymerisation a balance between the complexation ability of styrene and the insertion ability of methyl acrylate results in a 1:1 co-polymer.

