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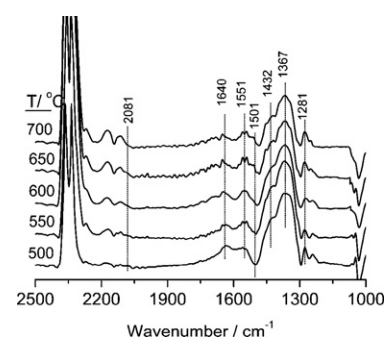
Articles

Jianjun Guo, Hui Lou, Liuye Mo, Xiaoming Zheng

Journal of Molecular Catalysis A: Chemical 316 (2010) 1

The reactivity of surface active carbonaceous species with CO₂ and its role on hydrocarbon conversion reactions

MgAl₂O₄ allows an effective way for CO₂ adsorption and activation through the formation of formate/carbonate type species. CH_x (x = 1–3) are the intermediates of methane activation on Ni particles and preferably diffuse from the metal to the interference of Ni and the supports and promote the adsorbed CO₂ species to decompose and release CO through formate/carbonate type intermediates.

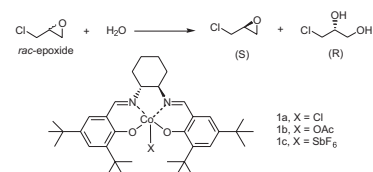


Surbhi Jain, Krishnan Venkatasubbaiah, Christopher W. Jones, Robert J. Davis

Journal of Molecular Catalysis A: Chemical 316 (2010) 8

Factors influencing recyclability of Co(III)-salen catalysts in the hydrolytic kinetic resolution of epichlorohydrin

The recyclability of Co(III)-salen catalysts for the hydrolytic kinetic resolution of racemic epichlorohydrin is a strong function of the counterion of the Co(III)-salen catalyst. The nature of the counterion determines whether the HKR reaction follows primarily a bimetallic or monometallic reaction path, which significantly affects catalyst recyclability.

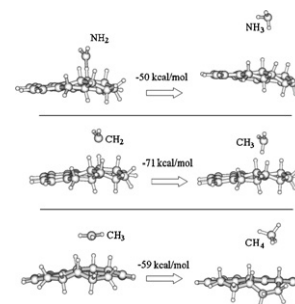


L.S. Rodríguez, F. Ruetter, M. Sánchez, C. Mendoza

Journal of Molecular Catalysis A: Chemical 316 (2010) 16

Interstellar catalysis: Formation of small molecules on a graphitic flake

The formation of molecules of the type XH_n where X is H, C, N and O and n=1–4, on the hydrogenated surface of a polycyclic aromatic hydrocarbon flake (coronene) has been examined in detail with the CATIVIC parametric quantum chemical code. We find that the reactions of atoms and small molecules with the hydrogenated coronene surface in most cases must overcome relatively high energy barriers in order to lead to reaction products.

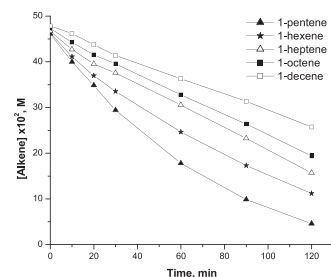


N. Sudheesh, Sumeet K. Sharma, Ram S. Shukla, Raksh V. Jasra

Journal of Molecular Catalysis A: Chemical 316 (2010) 23

Investigations on the kinetics of hydroformylation of 1-hexene using $\text{HRh}(\text{CO})(\text{PPh}_3)_3$ encapsulated hexagonal mesoporous silica as a heterogeneous catalyst

The hydroformylation of linear alkenes by a heterogeneous catalyst system, $\text{HRh}(\text{CO})(\text{PPh}_3)_3$ encapsulated into the pores of HMS acting as nanophase reactor, indicated that the rates were decreased on increasing the chain length. In the kinetics of a representative alkene, 1-hexene the rates were influenced on increasing, 1-hexene concentration, catalyst amount, temperature and partial pressures of CO and H_2 .



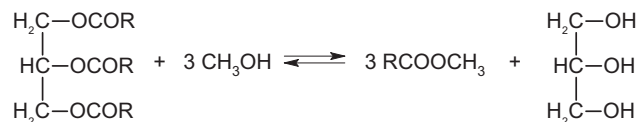
Time dependent consumption of alkenes during the reaction at alkene = 47.6×10^2 M, catalyst = 100 mg, $p_{\text{CO}} = 20$ bar, $p_{\text{H}_2} = 20$ bar, $T = 80^\circ\text{C}$, Toluene = 50mL.

A. Zieba, L. Matachowski, J. Gurgul, E. Bielańska, A. Drelinkiewicz

Journal of Molecular Catalysis A: Chemical 316 (2010) 30

Transesterification reaction of triglycerides in the presence of Ag-doped $\text{H}_3\text{PW}_{12}\text{O}_{40}$

Transesterification with methanol was studied for natural oil, castor oil and triacetin, a model compound in the presence of 12-tungstophosphoric acid and $\text{Ag}_x\text{H}_{3-x}\text{PW}_{12}\text{O}_{40}$ salts with Ag-content $x = 0.5$ up to $x = 3$. The activity data obtained under homogeneous and heterogeneous catalysis are compared.

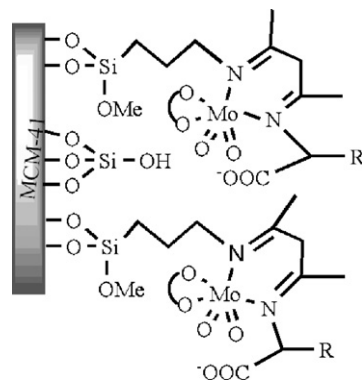


M. Masteri-Farahani

Journal of Molecular Catalysis A: Chemical 316 (2010) 45

Investigation of catalytic activities of new heterogeneous molybdenum catalysts in epoxidation of olefins

Incorporation of amino acid Schiff base ligands via reaction of acacAmpMCM-41 with different amino acids and subsequent treatment with $\text{MoO}_2(\text{acac})_2$ affords a new class of heterogeneous molybdenum catalysts for oxidation of olefins with high activity and selectivity toward the formation of the corresponding epoxides.

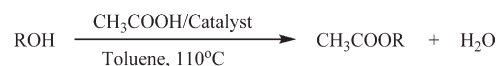


Lilian Osiglio, Gustavo Romanelli, Mirta Blanco

Journal of Molecular Catalysis A: Chemical 316 (2010) 52

Alcohol acetylation with acetic acid using borated zirconia as catalyst

The acetylated product yield in the alcohol acetylation correlates with the acid strength of the borated zirconia, which depends on the characteristics acquired in the solids through variation of oxide precursor concentration, boron concentration and calcination temperature.

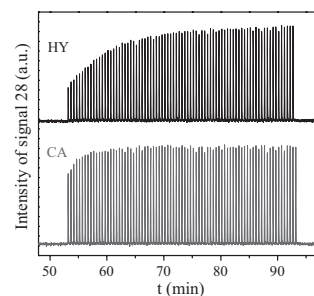


Yi Liu, Cun Wen, Yun Guo, Guanzhong Lu, Yanqin Wang

Journal of Molecular Catalysis A: Chemical 316 (2010) 59

Effects of surface area and oxygen vacancies on ceria in CO oxidation: Differences and relationships

The key factors and their relationship in CO oxidation were found on CeO₂ by comparing the activities of two kinds of CeO₂ in CO oxidation. Both surface area and surface oxygen vacancies play crucial role in CO oxidation because they influence the rate-determining step—the lattice oxygen extraction.

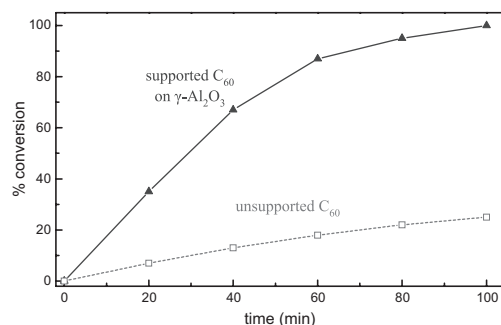


Manolis D. Tzirakis, John Vakros, Loukia Loukatzikou, Vasilis Amargianitakis, Michael Orfanopoulos, Christos Kordulis, Alexis Lycourghiotis

Journal of Molecular Catalysis A: Chemical 316 (2010) 65

γ -Alumina-supported [60]fullerene catalysts: Synthesis, properties and applications in the photooxidation of alkenes

The immobilization of C₆₀ on the surface of γ -Al₂O₃ increases considerably its catalytic activity for the photooxidation of alkenes.

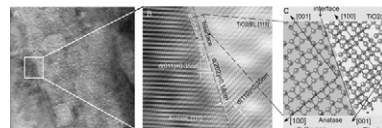


Zhanfeng Zheng, Hongwei Liu, Jianping Ye, Jincui Zhao, Eric R. Waclawik, Huaiyong Zhu

Journal of Molecular Catalysis A: Chemical 316 (2010) 75

Structure and contribution to photocatalytic activity of the interfaces in nanofibers with mixed anatase and TiO₂(B) phases

The interface in mixed phase titania nanofibers is built up by joining (2 0 2) of anatase and (2 0 2) of TiO₂(B). The two surfaces are similar in d-spaces \sim 0.18 nm. Bonding between the two phases reduces overall energy by removing surface energy associated with unsatisfied bonds. Moreover, such an interface structure provides explanation to the better photocatalytic activity of the mixed-phase nanofibers, compared with that of the mechanical mixtures with a similar phase composition.

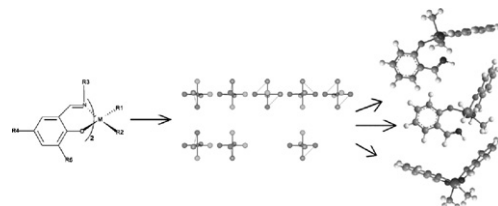


Zygmunt Flisak

Journal of Molecular Catalysis A: Chemical 316 (2010) 83

Theoretical study of isomerism in phenoxyimine-based precursors of coordinative olefin polymerization catalysts

Bis(phenoxyimine) group-4-metal complexes form eight isomeric structures. The stability of catalytically important isomers is studied by means of DFT. The factors that influence the isomeric preferences have been identified and discussed. Among them, the nature of the substituents at the nitrogen atom plays the most important role.

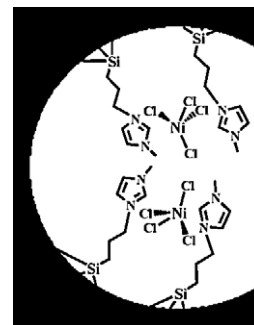


**Gang Liu, Minqiang Hou, Jiyuan Song,
Zhaofu Zhang, Tianbin Wu, Buxing Han**

Journal of Molecular Catalysis A: Chemical 316 (2010) 90

Ni²⁺-containing ionic liquid immobilized on silica: Effective catalyst for styrene oxidation with H₂O₂ at solvent-free condition

Ni²⁺-containing ionic liquid N-3-(3-triethoxysilylpropyl)-1-methyl imidazolium chloride immobilized on silica can catalyze styrene oxidation with H₂O₂ to produce benzaldehyde effectively under solvent-free condition. The unique advantage of the catalyst was that the reaction could be carried out at solvent-free condition. This advantage resulted mainly from the fact that both of the reactants, styrene and H₂O₂, are miscible with the IL, and the Ni²⁺ was coordinated by the immobilized IL that allowed both reactants to access to active sites of the catalyst effectively.

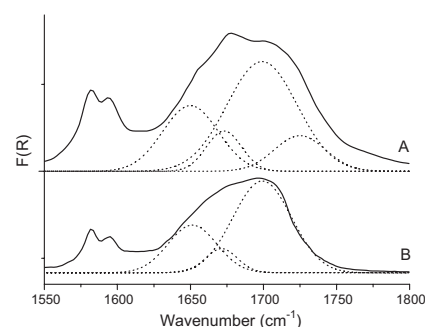


A.G. Potapov, G.D. Bukatov, V.A. Zakharov

Journal of Molecular Catalysis A: Chemical 316 (2010) 95

DRIFTS study of the interaction of the internal donor in TiCl₄/di-n-butyl phthalate/MgCl₂ catalysts with AlEt₃ cocatalyst

The internal donors form several types of complexes on the MgCl₂ support surface in supported Ziegler-Natta catalysts. A part of the internal donors is removed from the catalysts by AlEt₃ cocatalyst. IR-spectroscopy of diffuse reflection (DRIFTS) was used to study the interaction of the DBP/MgCl₂ support and TiCl₄/DBP/MgCl₂ catalysts (where DBP—di-n-butyl phthalate) with AlEt₃ cocatalyst. DRIFT spectra of DBP adsorbed on the MgCl₂ support (before (A) and after (B) interaction with AlEt₃) demonstrate effect of AlEt₃ on the distribution of DBP complexes on the MgCl₂ surface.

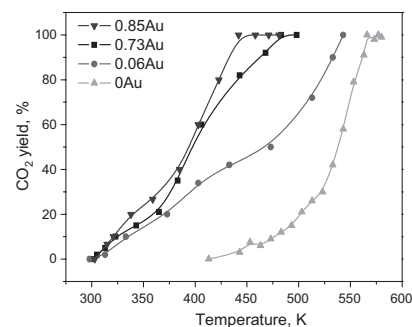


**Yanbing Zhang, Yuenian Shen, Xuzhuang Yang,
Shishan Sheng, Tana Wang, Moses F. Adebajo,
Huaiyong Zhu**

Journal of Molecular Catalysis A: Chemical 316 (2010) 106

Gold catalysts supported on the mesoporous nanoparticles composed of zirconia and silicate for oxidation of formaldehyde

Gold was loaded onto porous nanocomposite of ZrO₂ and silicate by deposition-precipitation. The resulting Au/ZrO₂-nanocomposites are superior catalysts for oxidizing formaldehyde from indoor air at moderate temperature. The analysis of temperature program desorption and temperature program surface reaction reveals that HCHO molecules strongly adsorb on the gold species in the samples at ambient temperature and convert rapidly into formate species, which react with adsorbed oxygen molecules.

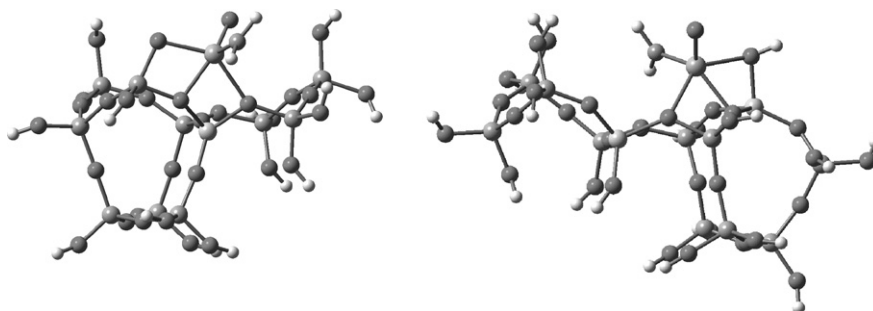


Jarosław Handzlik

Journal of Molecular Catalysis A: Chemical 316 (2010) 106

Computational study of the properties and metathesis activity of Mo methylenes species in HZSM-5 zeolite

Cluster models of Mo methylenes centres in HZSM-5 are investigated with DFT. The cycloaddition of ethene to the Mo methylenes centre is almost barrierless. The cycloreverse step involves a relatively high energy barrier for the Mo centre with one Al site in the vicinity, whereas the barrier is low for the model with two Al sites.

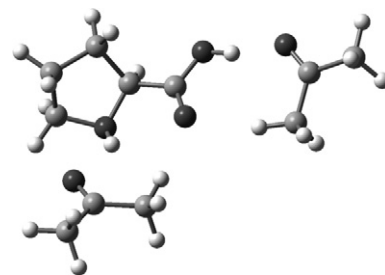


**Gang Yang, Zhiwei Yang, Lijun Zhou,
Rongxiu Zhu, Chengbu Liu**

Journal of Molecular Catalysis A: Chemical 316 (2010) 112

A revisit to proline-catalyzed aldol reaction: Interactions with acetone and catalytic mechanisms

The enamine structure mediates the proline-catalyzed aldol reaction. On basis of conformational studies, all the plausible mechanisms of enamine formation were considered. Two of them were found to be the most probable, where the transition states are geometrically stable and energy barriers are much lower compared with those reported by Boyd et al.

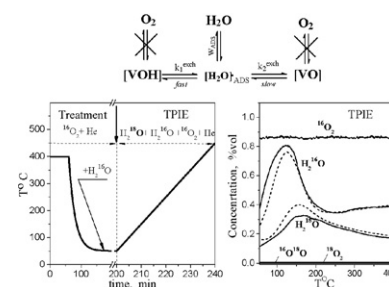


**E.M. Sadovskaya, V.B. Goncharov, Yu.K. Gulyaeva,
G.Ya. Popova, T.V. Andrushkevich**

Journal of Molecular Catalysis A: Chemical 316 (2010) 118

Kinetics of the $H_2^{18}O/H_2^{16}O$ isotope exchange over vanadia–titania catalyst

The ^{18}O exchange between H_2O , O_2 at monolayer vanadia–titania catalyst have been investigated in isothermic (200 °C) and thermo programmed (50–500 °C) conditions. TPIE in the $0.45\%H_2^{18}O + 0.15\%H_2^{16}O + 0.9\%^{16}O_2 + He$ flow (solid lines – experiment, dashed lines – calculation).

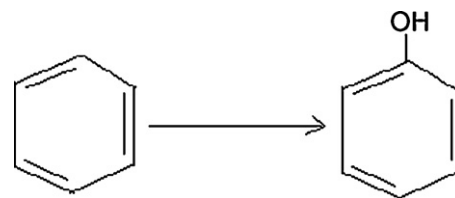


N.K. Renuka

Journal of Molecular Catalysis A: Chemical 316 (2010) 126

A green approach for phenol synthesis over Fe^{3+}/MgO catalysts using hydrogen peroxide

An efficient green route for the synthesis of phenol from benzene has been reported over Fe^{3+}/MgO catalysts under mild conditions using H_2O_2 as the oxidant. Fe^{3+}/MgO catalysts are prepared and well characterized using EDX, XRD, FTIR, surface area analysis pore volume determination and UV–vis diffuse reflectance studies. Phenol was exclusively obtained as the product.

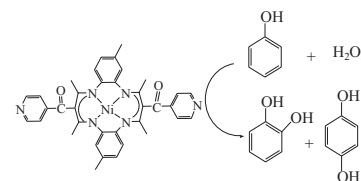


**Vipin Kumar Bansal, Pompozhi Protasis
Thankachan, Rajendra Prasad**

Journal of Molecular Catalysis A: Chemical 316 (2010) 131

Catalytic and electrocatalytic wet oxidation of phenol using two new nickel(II) tetraazamacrocyclic complexes under heterogeneous conditions

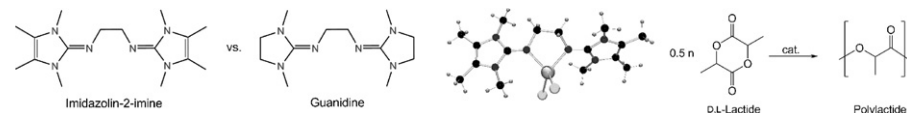
Two new Ni (II) tetraazamacrocyclic complexes have been synthesized and characterized. Their catalytic effects on electrochemical oxidation and regioselective chemical oxidation of phenol by H_2O_2 are also described. Effects of various parameters like temperature, amount of catalyst, amount of oxidant, effect of reaction media and time on the overall conversion as well as product selectivity have been investigated.



Janna Börner, Ulrich Flörke, Thomas Glöge, Thomas Bannenberg, Matthias Tamm, Matthew D. Jones, Artjom Döring, Dirk Kuckling, Sonja Herres-Pawlis

Journal of Molecular Catalysis A: Chemical 316 (2010) 139

New insights into the lactide polymerisation with neutral N-donor stabilised zinc complexes: Comparison of imidazolin-2-imine vs. guanidine complexes

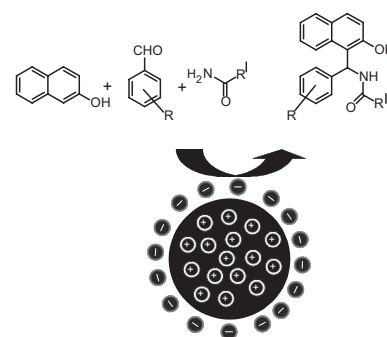


Gajanan Rashinkar, Rajashri Salunkhe

Journal of Molecular Catalysis A: Chemical 316 (2010) 146

Ferrocene labelled supported ionic liquid phase (SILP) containing organocatalytic anion for multi-component synthesis

Ferrocene labelled supported ionic liquid phase (SILP) catalyst containing L-prolinate anion has been synthesized. The SILP catalyst showed TON in the range of 1240–1740 and TOF in the range of 1.62–4.29 h⁻¹ in the multi-component synthesis of 1-amidoalkyl-2-naphthols.

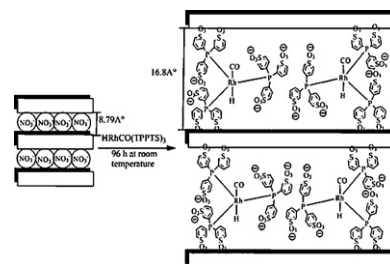


Sumeet K. Sharma, Parimal A. Parikh, Raksh V. Jasra

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Hydroformylation of alkenes using heterogeneous catalyst prepared by intercalation of HRh(CO)(TPPTS)₃ complex in hydrotalcite

The intercalation of HRh(CO)(TPPTS)₃ complex into interlayer space of hydrotalcite was carried out to prepared an eco-friendly heterogeneous catalyst for hydroformylation of alkenes. The catalyst showed excellent activity for hydroformylation of linear alkenes of varied carbon number from C₅ to C₁₃ as well as cyclic alkenes.



Chun-Hung Huang, I-Kai Wang, Yu-Ming Lin, Yao-Hsuan Tseng, Chun-Mei Lu

Journal of Molecular Catalysis A: Chemical 316 (2010) 163

Visible light photocatalytic degradation of nitric oxides on PtO_x-modified TiO₂ via sol-gel and impregnation method

The 1% PtO_x-modified TiO₂ by sol-gel process or impregnation method, with PtO–PtO₂ mixed valence states analyzed by XPS, promoted obviously visible light activity on degradation of NO_x. The PtO_x was not only considered to act as a sensitizer to respond to the visible light, but also advanced the total oxidation of NO and NO₂ to NO₃⁻.

