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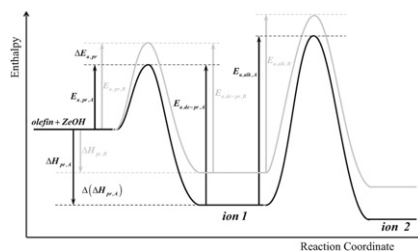
Articles

**Ionel Craciun, Marie-Françoise Reyniers,
Guy B. Marin**

*Journal of Molecular Catalysis A: Chemical 277
(2007) 1*

Effects of acid properties of Y zeolites on the liquid-phase alkylation of benzene with 1-octene: A reaction path analysis

The liquid phase alkylation of benzene with 1-octene was investigated over three USY zeolites with bulk Si/Al ratios of 6, 13 and 30, at temperatures ranging from 343 K to 373 K, benzene/1-octene feed molar ratios ranging from 1 to 10 and 1-octene conversions between 10 and 99%. The catalytic activity increases with increasing Si/Al ratio while the selectivities are not affected. The higher rates observed for the catalyst with the higher average acid strength can be traced back to a decrease in the activation energy for the protonation step leading to an increased concentration of carbenium ions on the catalyst surface that compensates for the higher activation energies for the deprotonation and alkylation steps. The constant selectivities are explained by a similar dependency of the different elementary steps on the acid site strength.

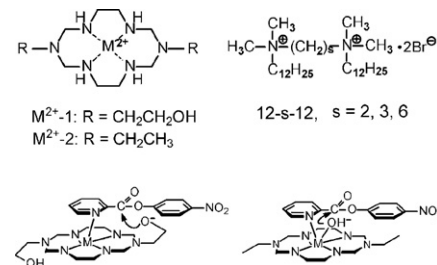


**Ling-Guang Qiu, Xia Jiang, Li-Na Gu,
Gang Hu**

*Journal of Molecular Catalysis A: Chemical 277
(2007) 15*

Gemini metallomicellar catalysis: Hydrolysis of *p*-nitrophenyl picolinate catalyzed by Cu(II) and Ni(II) complexes of macrocyclic ligands in gemini surfactant micelles

Catalytic hydrolysis of *p*-nitrophenyl picolinate (PNPP) in metallomicelle systems containing gemini surfactants 12-*s*-12 and metal complexes of macrocyclic ligands was investigated. Gemini metallomicellar systems were found to exhibit more efficient activities for hydrolysis of PNPP than those containing conventional surfactant dodecyltrimethylammonium bromide (DTAB), and metal complexes of macrocyclic ligand **1** bearing pendant hydroxyl groups show higher catalytic activities than corresponding complexes of **2** without hydroxyl group.

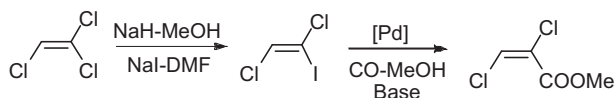


**Sylvain Pellegrini, Yves Castanet,
André Mortreux**

*Journal of Molecular Catalysis A: Chemical 277
(2007) 21*

Indirect palladium catalysed methoxycarbonylation of trichloroethylene

Methoxycarbonylation of trichloroethylene into methyl dichloroacrylate catalysed by PdCl₂(PPh₃)₂ was achieved via its conversion into iododichloroethylene.

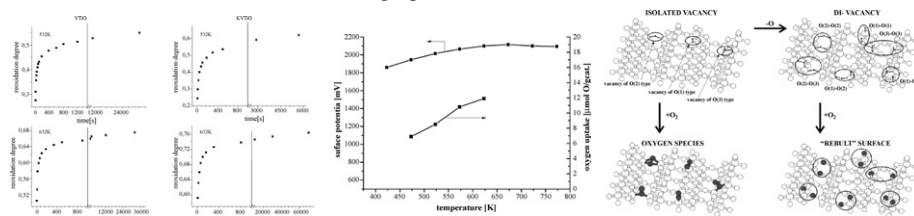


**J. Ślarczyński, R. Grabowski, A. Kozłowska,
R. Tokarz-Sobieraj, M. Witko**

Journal of Molecular Catalysis A: Chemical 277
(2007) 27

Interaction of oxygen with the surface of vanadia catalysts

The kinetics of the reoxidation of the reduced VO_x/TiO_2 catalysts was studied. It was found that oxygen does not adsorb in form of ad-atoms on the fully oxidized surface of the catalyst but re-oxidizes oxygen vacancies. The oxygen vacancies formed are quickly replenished with oxygen from the gaseous phase at temperatures above 473 K. On the basis of the surface potential measurements it was concluded that above 550 K the nucleophilic oxygen $\text{O}_{(s)}^{2-}$ is the dominant form of oxygen on the surface of the catalyst. The results of the quantum-chemical calculations were supported by experimental findings. Implications of these results on the mechanism reactions of the ODH of propane were discussed.

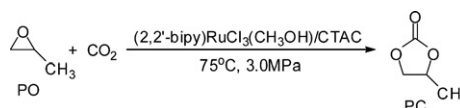


Zhanwei Bu, Gang Qin, Shaokui Cao

Journal of Molecular Catalysis A: Chemical 277
(2007) 35

A ruthenium complex exhibiting high catalytic efficiency for the formation of propylene carbonate from carbon dioxide

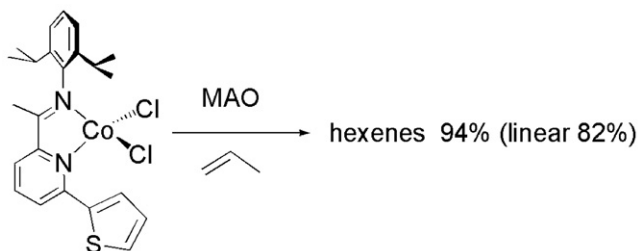
A highly efficient catalyst composed of $(2,2'\text{-bipy})\text{RuCl}_3(\text{CH}_3\text{OH})$ and cetyltrimethylammonium chloride (CTAC) is reported for the first time for the formation of propylene carbonate (PC) from carbon dioxide and propylene oxide (PO) under mild conditions (75 °C, 3.0 MPa). The catalyst can be easily recovered and reused several times without appreciable loss of catalytic activity.



**Claudio Bianchini, Giuliano Giambastiani,
Itzel Guerrero Rios, Andrea Meli,
Anna M. Segarra, Alessandro Toti,
Francesco Vizza**

Journal of Molecular Catalysis A: Chemical 277
(2007) 40

Regioselective propylene dimerization by tetrahedral (imino)pyridine Co^{II} dichloride complexes activated by MAO

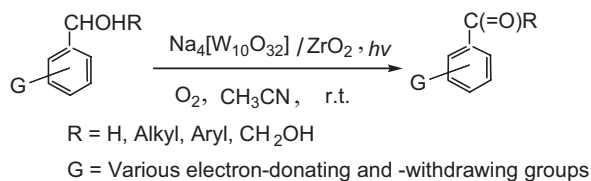


Saeid Farhadi, Zohreh Momeni

Journal of Molecular Catalysis A: Chemical 277
(2007) 47

Zirconia-supported sodium decatungstate ($\text{Na}_4\text{W}_{10}\text{O}_{32}/\text{ZrO}_2$): An efficient, green and recyclable photocatalyst for selective oxidation of activated alcohols to carbonyl compounds with O_2

Zirconia-supported sodium decatungstate, $\text{Na}_4\text{W}_{10}\text{O}_{32}/\text{ZrO}_2$, was prepared via a sol-gel technique and used as a green and recyclable heterogeneous photocatalyst for aerobic oxidation of a variety of activated alcohols into the corresponding carbonyl compounds.

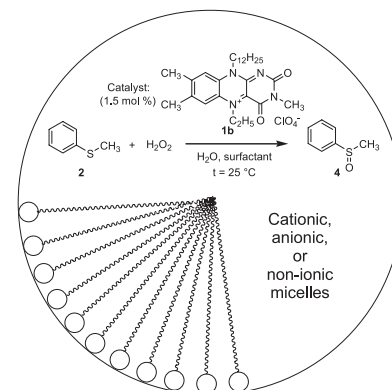


**Lenka Baxová, Radek Cibulka,
František Hampel**

Journal of Molecular Catalysis A: Chemical 277 (2007) 53

Organocatalytic sulfoxidation in micellar systems containing amphiphilic flavinium salts using hydrogen peroxide as a terminal oxidant

Amphiphilic flavinium salt **1b** solubilized in various types of micelles catalyzes the chemoselective oxidation of thioanisole (**2**) to sulfoxide **4**. Reaction rates strongly depended on the type of micellar matrix and on the pH value. In our experiments, micelles favoured the catalytic process rather than the non-catalyzed reaction. This effect was especially pronounced in cationic micelles, for which the non-catalyzed reaction was markedly suppressed.

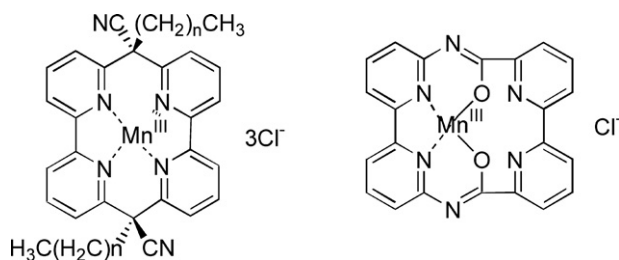


**Nirei Nakayama, Shinji Tsuchiya,
Shojiro Ogawa**

Journal of Molecular Catalysis A: Chemical 277 (2007) 61

Hydrocarbon oxidation with hydrogen peroxide and pentafluoriodosylbenzene catalyzed by unusually distorted macrocycle manganese complexes

An unsymmetrical macrocycle Mn complex with the unusually distorted structure was found to catalyze efficient oxidation of alkanes and aromatic compounds with hydrogen peroxide, and the selective epoxidation of alkenes was also observed. The specific epoxidation of alkenes catalyzed by the strained macrocycle Mn complexes consisting of two bipyridine moieties was found. The mechanism and the relationship between the macrocyclic structure and the oxidation products were discussed.

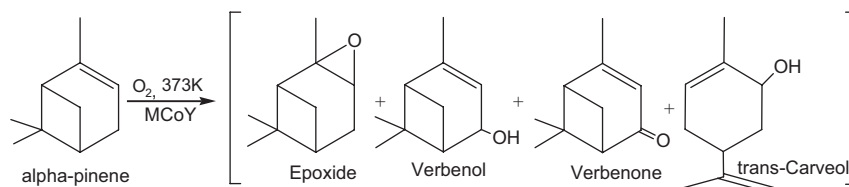


**Mallikarjun V. Patil, Mukesh K. Yadav,
Raksh V. Jasra**

Journal of Molecular Catalysis A: Chemical 277 (2007) 72

Catalytic epoxidation of α -pinene with molecular oxygen using cobalt(II)-exchanged zeolite Y-based heterogeneous catalysts

Cobalt-exchanged zeolite Y-based catalysts were studied for epoxidation of α -pinene with molecular oxygen using *N,N*-dimethylformamide (DMF) as a solvent at 373 K. The alkali and alkaline earth metal co-exchanged with cobalt Co(II) gives higher conversion than cobalt(II) alone. The best results were obtained using NaCsCoY20 with 47% α -pinene conversion and 61% epoxide selectivity at 80 psi pressure and 373 K temperature.

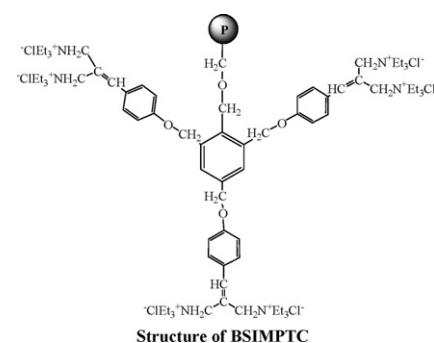


Eagambaram Murugan, Ayyanar Siva

Journal of Molecular Catalysis A: Chemical 277 (2007) 81

Effective Darzen's condensation of 4-nonanolide with 1,6-dibromohexan-2-one using new bead-shaped insoluble multi-site (six-site) phase transfer catalyst

A new bead-shaped insoluble polymer-supported multi-site phase transfer catalyst (BSIMPCTC), viz., 2,4,6-tris[4-(2,2'-bis(*N*-triethylammoniummethylene chloride) eth-1-ene) phenoxy]benzene has been synthesized and were characterized through spectroscopic and microscopic techniques. The catalytic efficiency of BSIMPCTC was examined by Darzen's condensation of 4-nonanolide with 1,6-dibromohexan-2-one reaction under pseudo-first order conditions.

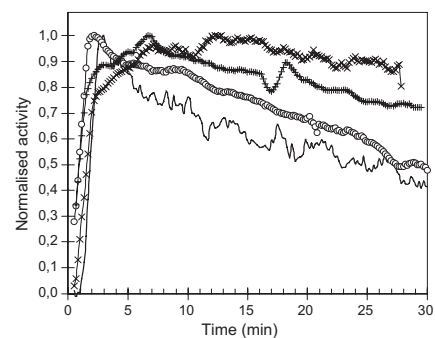


**João M. Campos, M. Rosário Ribeiro,
João Paulo Lourenço, Auguste Fernandes**

Journal of Molecular Catalysis A: Chemical 277 (2007) 93

Ethylene polymerisation with zirconocene supported in Al-modified MCM-41: Catalytic behaviour and polymer properties

Heterogeneous olefin polymerisation catalysts were prepared by combining zirconocene, with pure siliceous and Al-containing MCM-41 supports with different Si/Al ratios. Analysis of polymerisation activities and kinetic profiles led to a rationalisation on the effect of support Si/Al ratios and methods used for catalyst preparation over the catalytic behaviour of ethylene polymerisations. The formation or absence of fibrous morphology is linked with the polymerisation activities.

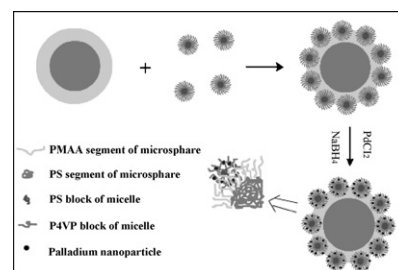


**Xiaowei Jiang, Guanwei Wei, Xu Zhang,
Wangqing Zhang, Peiwen Zheng, Fei Wen,
Linqi Shi**

Journal of Molecular Catalysis A: Chemical 277 (2007) 102

A strategy to facilitate reuse of palladium catalyst stabilized by block copolymer micelles

The Pd catalyst stabilized by polystyrene-*b*-poly(4-vinyl pyridine) micelle is anchored on surface of the core-shell polystyrene-*co*-poly(methyl acrylic acid) microspheres. The resultant raspberry-like colloid supported Pd catalyst, which shows similar activity to the catalyst stabilized by micelles and much improved recoverability, is a good alternative for Suzuki reaction.

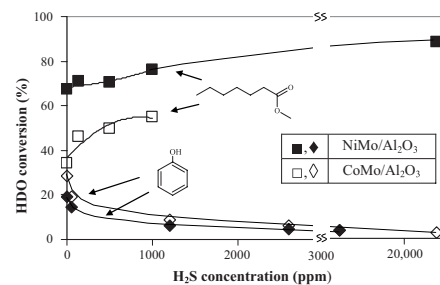


**O.İ. Şenol, E.-M. Ryymin, T.-R. Viljava,
A.O.I. Krause**

Journal of Molecular Catalysis A: Chemical 277 (2007) 107

Effect of hydrogen sulphide on the hydrodeoxygenation of aromatic and aliphatic oxygenates on sulphided catalysts

Effect of H₂S on the hydrodeoxygenation (HDO) of phenol was studied on sulphided NiMo/γ-Al₂O₃ and CoMo/γ-Al₂O₃ catalysts, and the results were compared with the effect of H₂S on the HDO of aliphatic oxygenates. H₂S inhibited the HDO of phenol by suppressing the direct hydrogenolysis reaction, but it enhanced the HDO of aliphatic oxygenates by enhancing acid-catalysed reactions of the oxygenates. The divergent effects were attributed to the different reaction mechanisms.

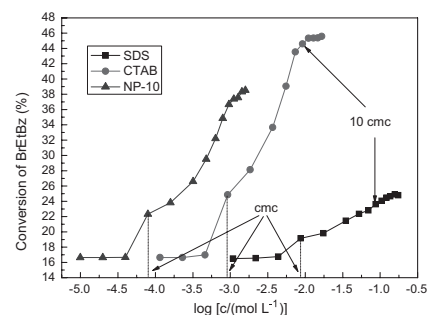


Qifa Liu, Ming Lu, Yeqing Li, Jiang Li

Journal of Molecular Catalysis A: Chemical 277 (2007) 113

Effect of organic electrolyte on chloromethylation of 2-bromoethylbenzene in micellar catalytic system

Surfactant micelles can catalyzed the chloromethylation of 2-bromoethylbenzene effectively and different types of surfactants have different catalytic abilities. A small amount of organic electrolyte tetrabutylammonium bromide was added into these micelles enhancing their catalytic abilities through a synergetic effect that allowed them to be much more active for the chloromethylation reaction.

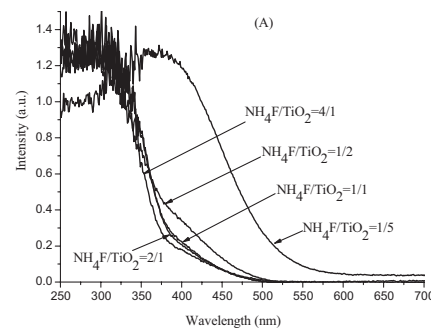


Yi Xie, Yuanzhi Li, Xiujuan Zhao

Journal of Molecular Catalysis A: Chemical 277 (2007) 119

Low-temperature preparation and visible-light-induced catalytic activity of anatase F–N-codoped TiO₂

UV–vis diffuse reflectance spectra shows that the F–N-codoping extends the absorbance spectra of TiO₂ into visible region and the intensity of the visible-light absorption decreases with increasing amount of starting reagent NH₄F.

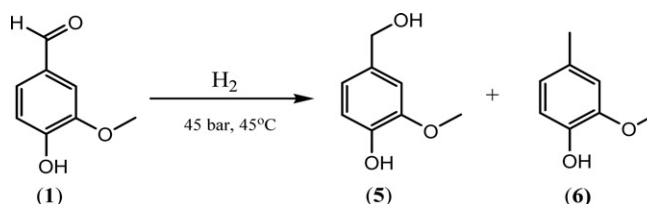


F.H. Mahfud, S. Bussemaker, B.J. Kooi, G.H. Ten Brink, H.J. Heeres

Journal of Molecular Catalysis A: Chemical 277 (2007) 127

The application of water-soluble ruthenium catalysts for the hydrogenation of the dichloromethane soluble fraction of fast pyrolysis oil and related model compounds in a two phase aqueous–organic system

The use of water-soluble homogeneous ruthenium catalysts (Ru–TPPTS, prepared *in situ* by reacting RuCl₃·3H₂O and tris(*m*-sulfonatophenyl)phosphine, TPPTS) to hydrogenate the dichloromethane soluble fraction of fast pyrolysis oil is reported. Significant reductions in the aldehyde content were observed at mild conditions (<70 °C, 45 bar hydrogen). Model studies with typical lignin derived compounds were performed and it was shown that vanillin (**1**) is hydrogenated to creosol (**6**) via the intermediate vanillylalcohol (**5**).

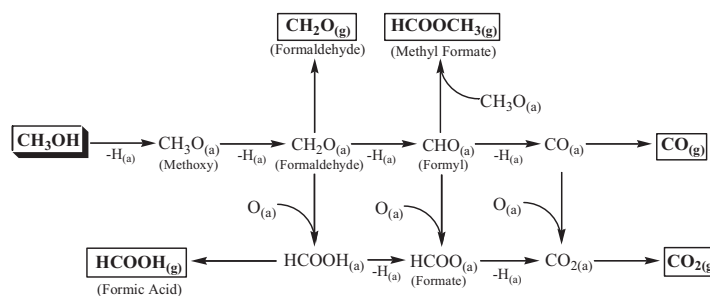


Ting C. Hsiao, Shawn D. Lin

Journal of Molecular Catalysis A: Chemical 277 (2007) 137

Effect of co-feed species on methanol conversion over Cu/ZnO/Al₂O₃ and its possible mechanism

Methanol conversion over a commercial Cu/ZnO/Al₂O₃ was examined with or without co-feed gas of H₂, H₂O or O₂ from 423 to 573 K. The steady-state activity and product selectivity can be shifted reversibly using different co-feed species. A reaction scheme is proposed accordingly to explain the effect of co-feed species on the reaction performance of Cu/ZnO.

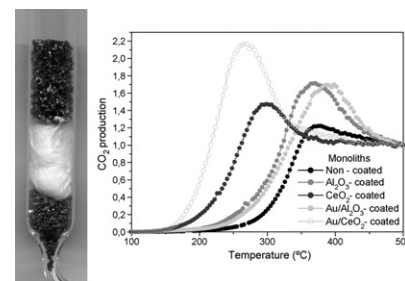


M.I. Domínguez, M. Sánchez, M.A. Centeno, M. Montes, J.A. Odriozola

Journal of Molecular Catalysis A: Chemical 277 (2007) 145

2-Propanol oxidation over gold supported catalysts coated ceramic foams prepared from stainless steel wastes

Reticulated ceramic foams prepared from steel making wastes were used as support for preparing Au/Al₂O₃ and Au/CeO₂ catalytic devices. The obtained catalytic systems are active to the 2-propanol oxidation reaction, presenting the Au/CeO₂-coated monolith the best catalytic results because of the combination of the oxidation capability of gold atoms with the redox properties of the ceria phase.

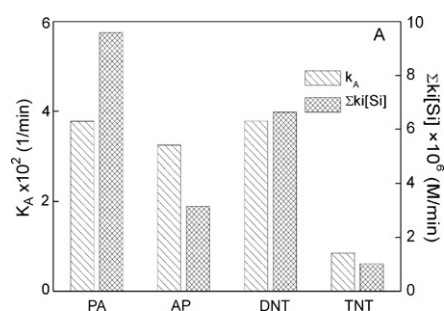


Ming-Jer Liou, Ming-Chun Lu

Journal of Molecular Catalysis A: Chemical 277 (2007) 155

Catalytic degradation of nitroaromatic explosives with Fenton's reagent

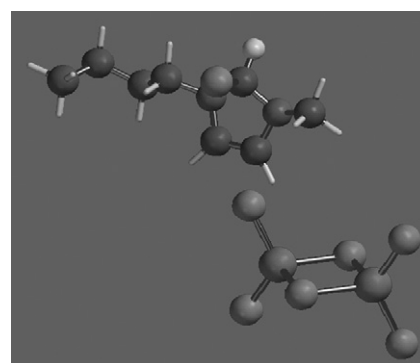
Oxidation of the nitroaromatic explosives namely, 2,4,6-trinitrophenol (PA), ammonium picrate (AP), 2,4-dinitrotoluene (DNT) and 2,4,6-trinitrotoluene (TNT) by Fenton's reagent has been investigated. Oxidation rate of the explosives in the Fenton process were in the following sequence: DNT > PA > AP > TNT. A half-life prediction model was proposed to prove the interference effect resulted from the oxidation intermediates.

**E.J. Angueira, M.G. White**

Journal of Molecular Catalysis A: Chemical 277 (2007) 164

Super acidic ionic liquids for arene carbonylation derived from dialkylimidazolium chlorides and MCl_3 (M = Al, Ga, or In)

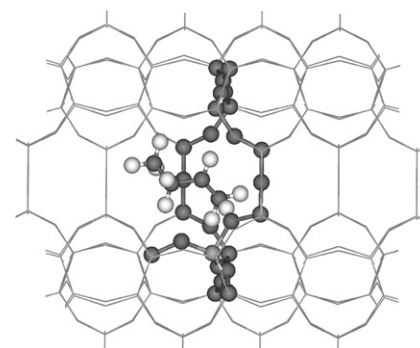
Ionic liquids, formed by combining 1 mol of 1-butyl-3-methyl-1H-imidazolium chloride, bim^+Cl^- , with 2 mol of a Group IIIA metal chloride (Al, Ga, In), were examined for toluene carbonylation reactivity to determine the effect for changing the M(III) cation. These ionic liquids were characterized for Brønsted acidity indirectly by ^{13}C NMR of labeled acetone, $CH_3-^{13}C=O-CH_3$. These results were explained by a mechanism where the Brønsted acidity of the ionic liquid was influenced by the strength of the Lewis acid: $M^{3+}Cl_3$.

**Piboon Pantu, Bundet Boekfa, Jumras Limtrakul**

Journal of Molecular Catalysis A: Chemical 277 (2007) 171

The adsorption of saturated and unsaturated hydrocarbons on nanostructured zeolites (H-MOR and H-FAU): An ONIOM study

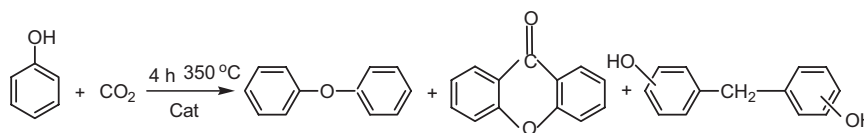
The ONIOM(MP2/6-31G(d,p):UFF//B3LYP/6-31G(d,p):UFF) was used to predict adsorption energies of light alkanes and alkenes in H-FAU and H-MOR. The extended zeolitic framework covering the nanocavity was essential for describing the confinement effect of the zeolites.

**Zhenhuan Li, Kunmei Su**

Journal of Molecular Catalysis A: Chemical 277 (2007) 180

The direct reaction between CO_2 and phenol catalyzed by bifunctional catalyst ZrO_2

The reaction between CO_2 and phenol had been investigated. The product distributions are influenced by the catalyst usage. With ZrO_2 as catalysts, the highest selectivity to 4-[4-hydroxybenzyl]phenol and 2-[2-hydroxybenzyl]phenol (HBP) was obtained, which may be ascribed to the bifunctional sites of catalyst. Metastable tetragonal ZrO_2 was suggested to be the active phase, and the formation of HBP might be relevant with bidentate carbonate on ZrO_2 surface.

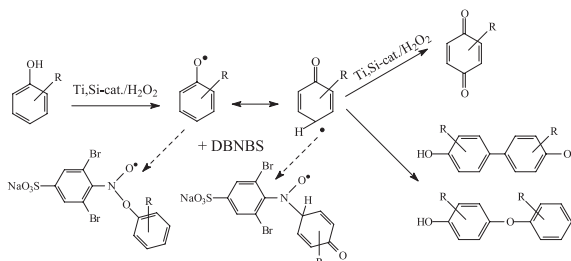


Olga V. Zalomaeva, Natalia N. Trukhan, Irina D. Ivanchikova, Alexander A. Panchenko, Emil Roduner, Eugenii P. Talsi, Alexander B. Sorokin, Vladimir A. Rogov, Oxana A. Kholdeeva

Journal of Molecular Catalysis A: Chemical 277 (2007) 185

EPR study on the mechanism of H₂O₂-based oxidation of alkylphenols over titanium single-site catalysts

The formation of aryloxy and hydroxyl radicals during the oxidation of 2,3,6-trimethylphenol and 2-methyl-1-naphthol with H₂O₂ in the presence of mesoporous titanium-silicate catalysts have been detected using EPR spectroscopic technique with spin traps, 3,5-dibromo-4-nitrosobenzene-sulfonic acid (DBNBS) and 5,5-dimethyl-1-pyrroline-*N*-oxide (DMPO). The EPR and by-product studies strongly support a homolytic oxidation mechanism.

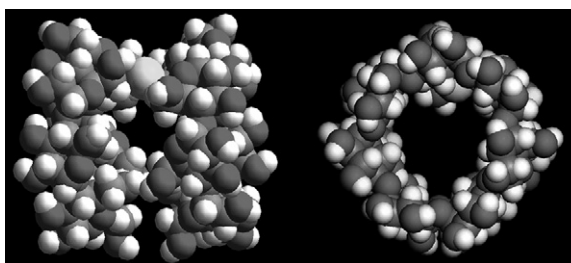


Zeyuan Dong, Kai Liang, Chunyu Wang, Xin Huang, Shizhong Mao, Xiangqiu Li, Jiayun Xu, Junqiu Liu, Guimin Luo, Jiaciong Shen

Journal of Molecular Catalysis A: Chemical 277 (2007) 193

A study of biomimetic system: Exploration of factors modulating the catalytic capacity of glutathione peroxidase mimics

Through the model of biomimetic two-substrate system we find that substrate binding is a key factor modulating the large rate accelerations of enzyme and difunctional recognition effectively accelerates the substrate specificity. Hydrophobic interactions are the primary driving forces during the enzyme-substrate recognition. Moreover, we also demonstrate that during catalysis the recognition manners of enzyme depend on the comparative affinities and concentrations of both substrates.

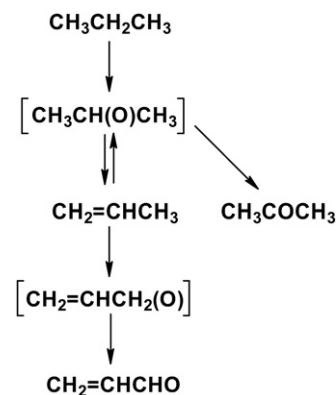


X.D. Yi, X.B. Zhang, W.Z. Weng, H.L. Wan

Journal of Molecular Catalysis A: Chemical 277 (2007) 202

Studies on the reaction pathways for the selective oxidation of propane to acrolein over MoPO/SiO₂ catalyst by IR spectroscopy

The reaction networks for propane selective oxidation to acrolein were proposed by using the IR spectroscopy studies the adsorbed species and gaseous species formed by adsorption of the reactant, possible intermediates or their probe molecules as well as the reaction products on the MoPO/SiO₂ catalyst and the transformation of these species at elevated temperature under vacuum and under O₂/He atmosphere.

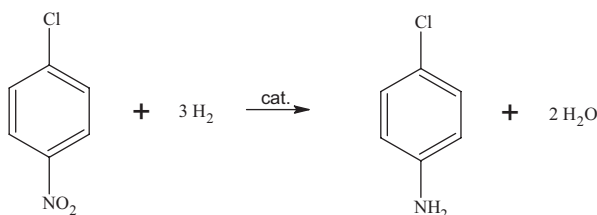


Xiao Xiang Han, Qing Chen, Ren Xian Zhou

Journal of Molecular Catalysis A: Chemical 277 (2007) 210

Study on the hydrogenation of *p*-chloronitrobenzene over carbon nanotubes supported platinum catalysts modified by Mn, Fe, Co, Ni and Cu

PtM/CNTs (M = Mn, Fe, Co, Ni and Cu) catalyst can catalyze the hydrogenation of *p*-chloronitrobenzene in ethanol at 303 K and normal pressure. PtFe/CNTs catalyst exhibits the best catalytic activity (TOF is 0.47 s⁻¹), and PtMn/CNTs catalyst exhibits the highest yield of *p*-CAN (98.5 mol%).

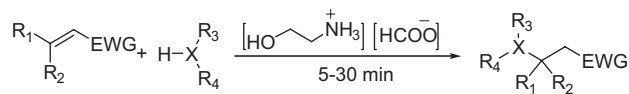


Yogesh O. Sharma, Mariam S. Degani

Journal of Molecular Catalysis A: Chemical 277 (2007) 215

Green and mild protocol for hetero-Michael addition of sulfur and nitrogen nucleophiles in ionic liquid

Comparatively novel and cost-effective ethanolamine based ionic liquid was utilized as alternative reaction medium as well as catalyst for synthetically important hetero-Michael reaction. The ionic liquid was compatible with various aromatic sulfur nucleophiles, secondary nitrogen nucleophiles and activated olefins. Rate of reaction was increased significantly and the results obtained are comparable or better to the reported methods.



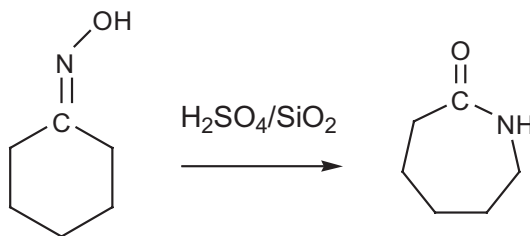
$R_1, R_2 = \text{H, Alkyl}$ $X = \text{N, S}$ When $X = \text{N}$; $R_3, R_4 = \text{Alkyl}$
When $X = \text{S}$; $R_3 = \text{aryl}$

N.C. Marziano, L. Ronchin, C. Tortato, A. Vavasori, C. Badetti

Journal of Molecular Catalysis A: Chemical 277 (2007) 221

Catalyzed Beckmann rearrangement of cyclohexanone oxime in heterogeneous liquid/solid system. Part 1: Batch and continuous operation with supported acid catalysts

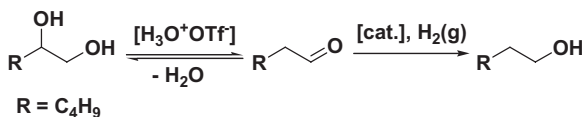
Beckmann rearrangement of cyclohexanone oxime to ϵ -caprolactam has been studied in heterogeneous liquid/solid system at room temperature and pressure. Preparation, characterization and reactivity of impregnated strong acids on solid support have been investigated, with particular attention to $\text{H}_2\text{SO}_4/\text{SiO}_2$ catalysts. Run conditions were as follows: T , 298 K; reaction volume, 20 ml; solvent, 1,2 dichloroethane; catalyst, 500 mg; cyclohexanone oxime concentration, 0.24–0.72 mol dm^{-3} .

**Ryan R. Dykeman, Kylie L. Luska, Michelle E. Thibault, Matthew D. Jones, Marcel Schlaf, Monther Khanfar, Nicolas J. Taylor, James F. Britten, Laura Harrington**

Journal of Molecular Catalysis A: Chemical 277 (2007) 233

Catalytic deoxygenation of terminal-diols under acidic aqueous conditions by the ruthenium complexes $[(\eta^6\text{-arene})\text{Ru}(\text{X})(\text{N} \cap \text{N})](\text{OTf})_n$, $\text{X} = \text{H}_2\text{O}$, H , $\eta^6\text{-arene} = p\text{-Me-}^i\text{Pr-C}_6\text{H}_4$, C_6Me_6 , $\text{N} \cap \text{N} = \text{bipy}$, phen , 6,6'-diamino-bipy, 2,9-diamino-phen, $n = 1, 2$). Influence of the *ortho*-amine substituents on catalytic activity

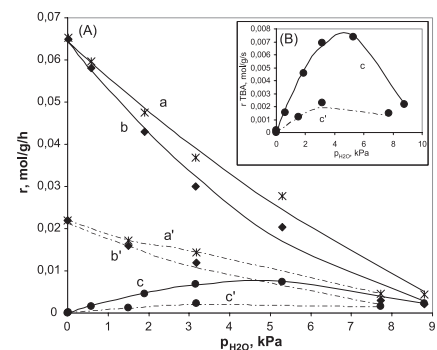
In sulfolane solvent at 110 °C under 5–7.5 MPa $\text{H}_2(\text{g})$ and the presence of free HOTf the complexes $[(\eta^6\text{-arene})\text{Ru}(\text{X})(\text{N} \cap \text{N})](\text{OTf})_n$ form acid and water-tolerant catalysts for the selective deoxygenation of terminal diols, notably 1,2-hexanediol, to the corresponding primary alcohol, i.e., 1-hexanol in up to 60% yield.

**A. Micek-Ilnicka**

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The effect of water vapour on kinetics of ethyl-*tert*-butyl ether (ETBE) and *tert*-butyl alcohol (TBA) synthesis in the gas phase on Wells–Dawson catalyst

The effect of water vapour in the feed on the synthesis of ethyl-*tert*-butyl ether (ETBE) produced from isobutene and ethanol was investigated. The kinetics of gas phase etherification and accompanying formation of *tert*-butyl alcohol (TBA) by Wells–Dawson acid heteropolyacid $\text{H}_6\text{P}_2\text{W}_{18}\text{O}_{62}$ as catalyst was determined at 40 °C. Water presence in the catalytic reactor inhibited the formation of ETBE and was introduced into the kinetic equation as independent additional factor.

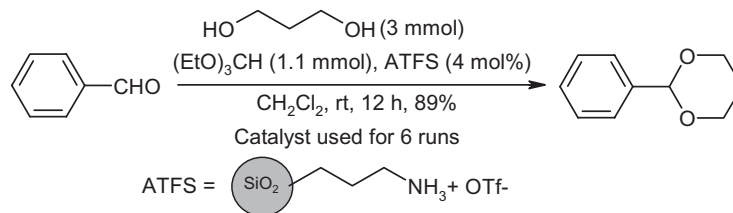


Babak Karimi, Maryam Ghoreishi-Nezhad

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Highly chemoselective acetalization of carbonyl compounds catalyzed by a novel recyclable ammonium triflate-functionalized silica

Various types of aldehydes as well as cyclic ketones were selectively converted to the corresponding 1,3-dioxanes in the presence of ethyl orthoformate, 1,3-propanediol and a catalytic amount of a novel ammonium triflate-functionalized silica ($\text{NH}_4^+\text{OTf}^-@ \text{SiO}_2$, ATFS) via an *in situ* acetal-exchange process. The catalyst can be recovered and reused for at least six reaction cycles without considerable loss of its reactivity.

**Asit K. Chakraborti**

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Comments on non-citation by H.R. Shaterian et al. [J. Mol. Catal. A: Chem. 272 (2007) 142–151] of the original work on the discovery of $\text{HClO}_4\text{-SiO}_2$

H.R. Shaterian

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Reply to the Letter to the Editor of Dr. Chakraborti: Comments on “Non-citation by H.R. Shaterian et al. of the original work on the discovery of $\text{HClO}_4\text{-SiO}_2$ ” [J. Mol. Catal. A: Chem. 272 (2007) 142–151]