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## Journal of Molecular Catalysis A: Chemical

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#### Articles

#### Abhishek Anan, Krishna K. Sharma, Tewodros Asefa

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Selective, efficient nanoporous catalysts for nitroaldol condensation: Co-placement of multiple site-isolated functional groups on mesoporous materials to introduce solid-base catalytic groups as well as secondary functional groups that can modify the dielectric environment of the pores. As grafting of a mixture of organosilanes in polar solvents resulted in site-isolated catalytic groups, selectivity was accompanied by high percentage conversion in <30 min.

The synthesis of selective, efficient multifunctional mesoporous catalysts for various p-substituted

hydrophilic or hydrophobic reactants in the Henry reaction was demonstrated. Grafting of 3-aminopropyl and 3-mercaptopropyl, methyl or ureidopropyl from a mixture of organosilanes in polar solvents has achieved

#### Selective, Efficient Trifunctional Nanoporous Catalysts



#### Alberto Acosta-Ramírez, David Morales-Morales, Juan Manuel Serrano-Becerra, Alma Arévalo, William D. Jones, Juventino J. García

Journal of Molecular Catalysis A: Chemical 288 (2008) 14

Study of the reactivity of 2-methyl-3-butenenitrile with Ni(0)-*N*-heterocyclic carbene complexes

A series of fluorinated and non-fluorinated *N*-heterocyclic carbenes were used for the catalytic isomerization of 2-methyl-3-butenenitrile, producing mainly a mixture of *E*- and *Z*-2M2BN, i.e., the C-H bond cleavage products.



#### Takao Sakamoto, Toshikatsu Takagaki, Aki Sakakura, Yasushi Obora, Satoshi Sakaguchi, Yasutaka Ishii

Journal of Molecular Catalysis A: Chemical 288 (2008) 19

Hydroxylation of benzene to phenol under air and carbon monoxide catalyzed by molybdovan-adophosphates



#### Venugopal Rajendran, Maw-Ling Wang

Journal of Molecular Catalysis A: Chemical 288 (2008) 23

Dichlorocarbene addition to allyl phenyl ether under phase-transfer catalysis conditions—A kinetic study The kinetics of phase-transfer catalysed dichlorocarbene addition to allyl phenyl ether has been investigated under biphase condition. The apparent rate constant of this reaction was obtained from experimental data. The effects of the reaction conditions, including agitation speed, amount of chloroform, quaternary ammonium salts, temperature and the amount of sodium hydroxide were investigated in detail.



Allyl Phenyl Ether



# D. Albanese, D. Landini, V. Lupi, M. Penso, D. Scaletti

The ring closing under solid–liquid phase-transfer catalysis (SL-PTC) conditions of hydroxysulfonamides **7**, bearing a leaving group in the *ortho* position of the aryl moiety, generates benzoxazines **4** in good to excellent yields. In the case of hydroxysulfonamides **7** bearing a bromine or iodine atom as a leaving group, a copper(I) salt is used.

Synthesis of 2-substituted 3,4-dihydro-2H-1, 4-benzoxazines through ligandless copper-catalyzed cyclization of hydroxysulfonamides under phasetransfer catalysis conditions

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#### Ganapati D. Yadav, Omprakash V. Badure

Journal of Molecular Catalysis A: Chemical 288 (2008) 33

Selective engineering in O-alkylation of *m*-cresol with benzyl chloride using liquid–liquid–liquid phase transfer catalysis

The conversion of liquid–liquid phase transfer catalysed (PTC) O-alkylation of cresols with benzyl chloride into liquid–liquid–liquid–liquid PTC leads to 100% selectivity to the ether at 50 °C and the reaction occurs in the middle phase.



#### Bo Xiao, Hongwei Hou, Yaoting Fan

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Syntheses and structural characteristics of copper(II)-organic polymers based on N-heterocyclic ligands: A study on the importance of steric factors in the design of potent catalysts

Two new Cu(II)-organic polymers containing coordinatively unsaturated metal sites are designed and synthesized as competent heterogeneous catalysts for the oxidative coupling of various substituted phenols in aqueous medium. It is suggested that the combination of the physical and chemical properties of inorganic and organic components can allow the achievement of the targeted polymeric materials furnishing unusual catalytic characters.



#### Ahmed K. Aboul-Gheit, Sahar M. Ahmed, Samia A. Hanafy

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Exchanged zeolites with transition metals of the first period as photocatalyts for *n*-hexadecane degradation

The photodegradation of *n*-hexadecane ( $n-C_{16}$ ) was tested using photocatalysts containing MOR, ZSM-5 or Y zeolites exchanged with ∼5.2 wt% V, Cr, Mn, Cu or Zn. Spectra examinations indicated retaining high crystallinity and the current-exchanged metals are present as isolated species. The photocatalytic degradation rate constant, *k*, and the adsorption coefficient,  $K_{ad}$ , were found to correlate with the metals atomic weights and their active cationic surface area.



#### Lucilene L. de Oliveira, Roberta R. Campedelli, Maria C.A. Kuhn, Jean-François Carpentier, Osvaldo L. Casagrande Jr.

Dimerization of ethylene in the presence of Ni(II) 5-membered chelate complexes based on tridentate nitrogen- or sulfur-bridged bis(pyrazolyl) ligands (NZN) (Z = N, S) activated with alkylaluminum (MAO or DEAC) proceeds with high activity and selectivity under moderate conditions.

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Highly selective nickel catalysts for ethylene oligomerization based on tridentate pyrazolyl ligands



#### David L. Trimm, Irene O.Y. Liu, Noel W. Cant

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The oligomerization of acetylene in hydrogen over Ni/SiO<sub>2</sub> catalysts: Product distribution and pathways

The reaction of acetylene–hydrogen mixtures over Ni/SiO<sub>2</sub> catalysts is found to proceed by chain growth with complete conversion at 140 °C to &sim;50% C<sub>2</sub>, &sim;20% C<sub>4</sub> and 30% C<sub>5</sub>+ products. The principal oligomers, exemplified for C<sub>6</sub> products, are the terminal and *cis*-linear alkenes together with 3-methyl branched pentenes and pentadienes, with much lesser amounts of 2-methyl and cyclic products.



#### Cathrin Welker, Noko S. Phala, John R. Moss, Michael Claeys, Eric van Steen

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Theoretical feasibility of CO-activation and Fischer-Tropsch chain growth on mono- and diatomic Ru complexes



DFT-calculations show that typical Fischer-Tropsch reactions may occur over di-atomic Ru-complexes,

whereas the energetics of reaction pathway over mono-atomic Ru-complexes are too high resulting in very

#### Contents

#### Yutaka Hitomi, Shinya Furukawa, Masakazu Higuchi, Tetsuya Shishido, Tsunehiro Tanaka

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Alkane hydroxylation catalyzed by a series of mononuclear nonheme iron complexes containing 4-nitropyridine ligands Catalytic oxidation of cyclohexane with  $H_2O_2$  was examined by using a series of iron(II) complexes supported by tris(2-pyridylmethyl)amine and its nitro-substituents as a catalyst. The introduction of nitro-groups retarded the generation of *cis*-oxohydroxo-iron(V) species, leading to a decrease in turnover number, and decreased the A/K ratio close to 1, probably through homolysis of the Fe-O bond of Fe(III)OOH species.



#### Fuat E. Celik, Henry Lawrence, Alexis T. Bell

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Synthesis of precursors to ethylene glycol from formaldehyde and methyl formate catalyzed by heteropoly acids Formaldehyde derived from different sources was carbonylated catalytically with methyl formate using silicotungstic acid, producing methyl glycolate and methyl methoxyacetate. Release of carbon monoxide from methyl formate was found to be slow, limiting productivity. The reducibility and softness of the Keggin unit, not acid strength, was used to explain the superior activity of silicotungstic acid over other common heteropolyacids and methanesulfonic acid.



#### Paolo Zucca, Carla Vinci, Francesca Sollai, Antonio Rescigno, Enrico Sanjust

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Degradation of Alizarin Red S under mild experimental conditions by immobilized 5,10,15,20tetrakis(4-sulfonatophenyl)porphine–Mn(III) as a biomimetic peroxidase-like catalyst Alizarin Red S oxidative degradation by  $H_2O_2$  in the presence of the catalyst prepared by immobilizing 5,10,15,20-tetrakis(4-sulfonatophenyl)porphine–Mn(III) on a modified silica support is described. The bleaching process was efficient and took place under very mild experimental conditions, mainly leading to phthalic acid. Some operational features of the catalytic reaction are described and a chemical mechanism for the bleaching is proposed.



Intermediates of biologically active 3,5-substituted indole derivatives have been successfully obtained by

rhodium-catalyzed domino hydroformylation /indolization of m-substituted-o-nitrocinnamal-dehyde diethyl

# M. Marchetti, S. Paganelli, D. Carboni, F. Ulgheri, G. Del Ponte

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acetals.

Synthesis of indole derivatives by domino hydroformylation/indolization of 2-nitrocinnamal-dehydes



#### Long Huang, Yulei Zhu, Chunfang Huo, Hongyan Zheng, Gang Feng, Chenghua Zhang, Yongwang Li

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Mechanistic insight into the heterogeneous catalytic transfer hydrogenation over Cu/Al<sub>2</sub>O<sub>3</sub>: Direct evidence for the assistant role of support

By the means of mechanical mixture of supported catalyst and its pure support, the support is demonstrated to play a remarkable assistant role in heterogeneous catalytic transfer hydrogenation between alkene and alcohol over Cu/Al<sub>2</sub>O<sub>2</sub>. The reaction results strongly suggest a bifunctional mechanism as follows: (Step 1) alcohols absorption, (Step 2) alcohols dehydrogenation with cooperation of Al<sub>2</sub>O<sub>2</sub> and Cu, (Step 3) reverse hydrogen spillover from  $Al_2O_3$  surface to metal phase, (Step 4) the alkene hydrogenation on metal phase.

The imidazole-modified silica (Silm) was used for immobilization of Mn(Br, TPP)Cl and Mn(TPP)Cl. These heterogeneous catalysts were used as biomimetic oxidation catalysts in alkene epoxidation and alkane hydroxylation with sodium periodate under agitation with magnetic stirring and ultrasonic irradiation. These new heterogenized catalysts could be reused several times without significant loss of their catalytic activity.

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Majid Moghadam, Valiollah Mirkhani,

Iraj Mohammdpoor-Baltork, Hadi Kargar

Shahram Tangestaninejad,

Silica supported Mn(Br, TPP)Cl and Mn(TPP)Cl as efficient and reusable catalysts for selective hydrocarbon oxidation under various reaction conditions: The effect of substituted bromines on the catalytic activity and reusability

### K.M. Parida, P. Mohapatra, John Moma, W.A. Jordaan, Mike S. Scurrell

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Effects of preparation methods on gold/titania catalysts for CO oxidation



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Corrigendum to "Carboxylation of benzene with CO and O<sub>2</sub> catalyzed by Pd(OAc)<sub>2</sub> and molybdovanadophosphates" [J. Mol. Catal. A: Chem. 282 (2008) 22-27]



1e

1f

1d







