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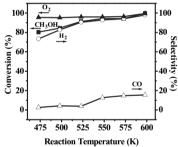
journal homepage: www.elsevier.com/locate/molcata

### Contents

Articles	
Ana Ison, Cheng Xu, G. Ken Weakley, David E. Richardson	The hydrocarbon-soluble coordination complex $[Fe(4,7-diphenyl-1,10-phenanthroline)_3](SO_3CF_3)_2$ (1) is an active catalyst for the autoxidation of cumene and cyclohexane. The activity of 1 in the autoxidation of cumene at 60 °C is comparable to that of tetra(pentafluorophenyl)porphyrin iron(III) chloride (2), a halogenated iron
Journal of Molecular Catalysis A: Chemical 293 (2008) 1	porphyrin with high autoxidation activity. The kinetic data have been fit by a mechanism in which the iron catalyst is activated by reaction with peroxide and the resulting active complex acts as a peroxide decomposi-
Catalytic autoxidations using tris-diimine iron(II) coordination complexes	tion catalyst producing chain-carrying radicals. The activity of 1 is also comparable to that of 2 in the autoxidation of cyclohexane at 135 °C. The utility of catalyst 1 is enhanced by its solubility in pure hydrocarbon substrates. DPP=4,7-diphenyl-1,10-phenanthroline
Ti-Cheng Ou, Feg-Wen Chang, L. Selva Roselin	Hydrogen production via partial oxidation of methanol was studied over Au–Cu/TiO, $(1-1 \text{ wt.\%})$ and Au/TiO, $(2 \text{ wt.\%})$ and 100 100 100 100 100 100 100 100 100 10
Journal of Molecular Catalysis A: Chemical 293 (2008) 8	Cu/TiO <sub>2</sub> (2 wt.%) catalysts. The Au–Cu/TiO <sub>2</sub> catalyst exhibits higher activity stability and selectivity towards the desired product. This $30$

Production of hydrogen via partial oxidation of methanol over bimetallic Au-Cu/TiO<sub>2</sub> catalysts

activity, stability and selectivity towards the desired product. This is due to Au-Cu interaction that creates smaller metal particles and stabilizes the active Au species for POM to produce hydrogen.



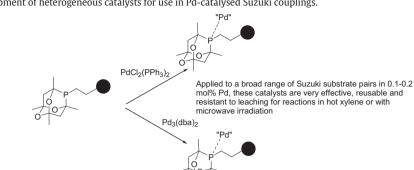


### Meritxell Guinó, Alice C. Sullivan, John R.H. Wilson

We report on the immobilisation of the phosphaadamantane function onto silica via an ethyl linker group and the development of heterogeneous catalysts for use in Pd-catalysed Suzuki couplings.

Journal of Molecular Catalysis A: Chemical 293 (2008) 25

Silicaethylphosphatrioxaadamantane—A new support for palladium catalysts and evaluation in Suzuki coupling reactions

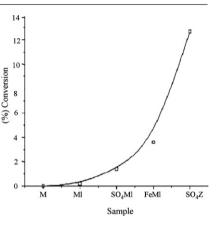


### Alcineia C. Oliveira, Nadine Essayem, Alain Tuel, Jean-Marc Clacens, Younes Ben Tâarit

Journal of Molecular Catalysis A: Chemical 293 (2008) 31

Comparative study of transformation of linear alkanes over modified mordenites and sulphated zirconia catalysts: Influence of the zeolite acidity on the performance of *n*-butane isomerization

Iron or sulphates impregnated on dealuminated mordenite showed an enhanced conversion in the transformation of *n*-butane to isobutane compared to non-dealuminated or dealuminated modernite. Fe or  $SO_4^{-2}$  species produce new active sites that promote the catalytic activity due to the highest strength of few sites and/or to the occurrence of an initial red-ox activation step over iron species. However, modified mordenites remain less active than conventional sulphated zirconia, used as reference catalyst.



### Praveen K. Tandon, Manisha Purwar, Satpal Singh, Nidhi Srivastava, Manish Srivastava

Journal of Molecular Catalysis A: Chemical 293 (2008) 39

Graphical separation of un-catalyzed and catalyzed reactions in iridium(III) catalyzed oxidation of cinnamaldehyde by cerium(IV) in aqueous acidic medium

Addition of catalyst changes the order of reaction in oxidant and its intercept gives the value of the rate of un-catalyzed reaction in Ir<sup>III</sup> catalyzed oxidation of cinnamaldehyde by Ce<sup>IV</sup> in acidic medium. Cerium(IV) is not reduced before the slow step with cinnamic acid as the oxidation product. Catalyzed path may be given as

- d[Ce <sup>IV</sup> ]	kK <sub>1</sub> K <sub>2</sub> [Ce <sup>IV</sup> ][S][Ir <sup>III</sup> ]		
dt	1+ K <sub>1</sub> K <sub>2</sub> [Ce <sup>IV</sup> ][S]		

O. Schwarz, D. Habel, O. Ovsitser, E.V. Kondratenko, C. Hess, R. Schomäcker, H. Schubert	Two preparation methods (wet saturation impregnation and ball-milling) were applied to produce $VO_x/\gamma$ -Al <sub>2</sub> O <sub>3</sub> materials with comparable physico-chemical and catalytic properties although	70	Impregnated catalysts O Ball-milled catalysts
Journal of Molecular Catalysis A: Chemical 293 (2008) 45	very different precursors were used. The calcination step during catalyst preparation was found to be essential for dispersing VO <sub>v</sub>	ivity [%]	· · · ·
Impact of preparation method on physico-chemical and catalytic properties of $VO_x/\gamma$ -Al <sub>2</sub> O <sub>3</sub> materials	species on the support material surface. A correlation between edge energies derived from UV/vis-DRS experiments and catalytic performance was established.	Propene select	• • •



Contents

### M. Badawi, L. Vivier, G. Pérot, D. Duprez

Journal of Molecular Catalysis A: Chemical 293 (2008) 53

Promoting effect of cobalt and nickel on the activity of hydrotreating catalysts in hydrogenation and isomerization of olefins

### Relative reactivity in hydrogenation: On sulfided CoMo and Mo catalysts :

On sulfided NiMo catalyst :

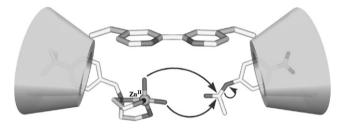
Promoting effect:In hydrogenation:CoIn isomerization:NiCo

### Ying-Hua Zhou, Meng Zhao, Ji-Hui Li, Zong-Wan Mao, Liang-Nian Ji

Journal of Molecular Catalysis A: Chemical 293 (2008) 59

Carboxylic ester hydrolysis catalyzed by a host–guest system constructed by cyclodextrin dimer and zinc complex

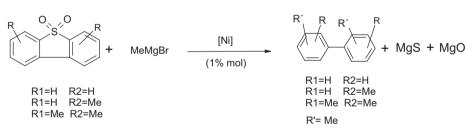
# A new $\beta$ -cyclodextrin dimer was synthesized and further assembled with a zinc complex containing a hydrophobic group as a new supramolecular system of catalyzing ester hydrolysis. Thermodynamic properties of the supramolecular complex in solution and kinetics of catalyzing *p*-nitrophenyl acetate hydrolysis were investigated and obtained very good consistent results in hydroxyl active species. Compared with an unassembled host or guest analogue, the supramolecular complex exhibits much higher catalytic activity.



## Alberto Oviedo, Jorge Torres-Nieto, Alma Arévalo, Juventino J. García

Journal of Molecular Catalysis A: Chemical 293 (2008) 65

Deoxydesulfurization of sulfones derived from dibenzothiophene using nickel compounds



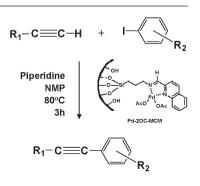
The use of catalytic amounts of compounds of the type [Ni(diphosphine)H], allowed the deoxydesulfurization

### Kenichi Komura, Hideki Nakamura, Yoshihiro Sugi

Journal of Molecular Catalysis A: Chemical 293 (2008) 72

Heterogeneous copper-free Sonogashira coupling reaction of terminal alkynes with aryl halides over a quinoline-2-carboimine palladium complex immobilized on MCM-41 Heterogeneous Sonogashira cross-coupling of terminal alkynes with aryl halides was studied over a quinoline-carboimine palladium complex immobilized on MCM-41 (Pd-2QC-MCM) as catalyst. Cross-coupling of phenyl acetylene with iodobenzene proceeded within 3 h at 80 °C by adding two-fold amount of piperidine in NMP solvent to afford tolane in excellent yield. Pd-2QC-MCM can be reused without significant loss of activity until 4th recycles.

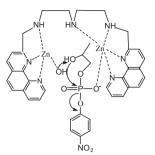
of dibenzothiophene-sulfones, quantitatively yielding biphenyls.



### XiangXia Wu, Hai Lin, Jie Shao, Huakuan Lin

Journal of Molecular Catalysis A: Chemical 293 (2008) 79

Study on kinetics and mechanism of dinuclear metal zinc(II) complexes in promoting the hydrolysis of 2-hydroxy-propyl-*p*-nitrophenyl phosphate (HPNP) Five multi-dentate ligands have been synthesized and characterized. The hydrolytic kinetics catalyzed by dinuclear complexes of Zn(II) with L1–L5 have been studied in aqueous solution at 298.2 ± 0.1 K, *I* = 0.10 mol dm<sup>-3</sup> KNO<sub>3</sub> at pH 7.0–8.5, respectively. The results showed that the catalytic effect of Zn<sub>2</sub>L3 was the best in the five dinuclear complexes for hydrolysis of 2-hydroxy-propyl-*p*-nitrophenyl phosphate (HPNP).

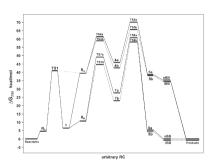


### Sławomir Ostrowski, Jan Cz. Dobrowolski

Journal of Molecular Catalysis A: Chemical 293 (2008) 86

Side-chain alkylation of toluene with propene over a basic catalyst. A DFT study

The toluene methyl group alkylation by propene was modeled by the B3LYP/6-311++G<sup>\*\*</sup> method. Two reaction paths are considered. The energy levels at Path A are always above those of Path B, whereas the essential barriers oppositely. We interpret Path A as describing the reaction in the bulk gas phase whereas Path B as describing the reaction at the metal surface.

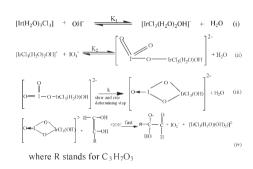


### Surya Prakash Singh, Ashok Kumar Singh, Ajaya Kumar Singh

Journal of Molecular Catalysis A: Chemical 293 (2008) 97

First and novel oxidation of D-fructose by potassium iodate using  $[IrCl_3(H_2O)_2OH]^-$  complex as a homogeneous catalyst in alkaline medium

The following general scheme is proposed for the first and novel oxidation of D-fructose by potassium iodate using  $[IrCl_3(H_2O)_2OH]^-$  complex as a homogeneous catalyst in alkaline medium to explain the observed experimental results:



### Masami Fukushima, Satoko Shigematsu

Journal of Molecular Catalysis A: Chemical 293 (2008) 103

Introduction of 5,10,15,20-tetrakis(4-hydroxyphenyl)porphine iron(III) into humic acid via formaldehyde polycondensation

