



## Journal of Molecular Catalysis A: Chemical

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### Contents

#### Articles

#### Ard C.J. Koeken, Leo J.P. van den Broeke, Berth-Jan Deelman, Jos T.F. Keurentjes

Journal of Molecular Catalysis A: Chemical 346 (2011) 1

Full kinetic description of 1-octene hydroformylation in a supercritical medium

▶ Mathematical model of kinetics of 1-octene hydroformylation in supercritical  $CO_2$ . ▶ The reaction is first order in hydrogen and rhodium. ▶ Increasing phosphine ligand concentration improves selectivity and activity. ▶ 1-Octene reaction order shifts from one to below zero with increasing concentration. ▶ Rhodium with trifluoromethylated phosphine allows for high turnover frequencies.



**ICATA** 

#### A. Aguirre-Gutiérrez, J.A. Montoya de la Fuente, J.A. de los Reyes, P. del Angel, A. Vargas

Journal of Molecular Catalysis A: Chemical 346 (2011) 12

Palladium effect over Mo and NiMo/alumina-titania sulfided catalysts on the hydrodesulfurization of 4,6-dimethyldibenzothiophene

# ▶ Pd was incorporated on the NiMo/AT in the oxidic phase. ▶ HRTEM results suggest that Pd and Ni are highly dispersed. ▶ Pd incorporation over the NiMo/AT sample increased the reaction rate by 30%. ▶ Pd promotes hydrogenation of intermediate products, increasing total conversion.



#### Helena Bergenudd, Mats Jonsson, Eva Malmström

▶ Iron complexes as mediators in normal and reverse ATRP of MMA in DMF. ▶ Electrochemical and polymerization properties are investigated. ▶ Strong indications of different iron species in normal and reverse ATRP. ▶ The nature of the ligand is not crucial for the polymerization outcome.

Journal of Molecular Catalysis A: Chemical 346 (2011) 21

Investigation of iron complexes in ATRP: Indications of different iron species in normal and reverse ATRP





#### Chuanzhi Sun, Lihui Dong, Wujiang Yu, Lichen Liu, Hao Li, Fei Gao, Lin Dong, Yi Chen

Journal of Molecular Catalysis A: Chemical 346 (2011) 30

Promotion effect of tungsten oxide on SCR of NO with NH<sub>3</sub> for the  $V_2O_5$ -WO<sub>3</sub>/Ti<sub>0.5</sub>Sn<sub>0.5</sub>O<sub>2</sub> catalyst: Experiments combined with DFT calculations

► The V–O–W bond forms when the vanadium oxide and tungsten oxide are co-impregnated on support.

▶ Brønsted acid sites are the main active sites for "NO + NH3 + O2" reaction. ▶ The acid strength of Brønsted acid and the reducibility of vanadium oxide species are not responsible for the high SCR activities. The excessive WO<sub>3</sub> cover the vanadium oxide species

leading to the decrease of the SCR activity. > DFT calculations are employed to elucidate the effect of WO<sub>3</sub>.



#### Abbas Teimouri, Alireza Najafi Chermahini

Journal of Molecular Catalysis A: Chemical 346 (2011) 40

An efficient and one-pot synthesis of 2,4,5trisubstituted and 1,2,4,5-tetrasubstituted imidazoles catalyzed via solid acid nano-catalyst

A one-pot, multicomponent methodology has been developed for the synthesis of 2,4,5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles catalyzed by clays, zeolite and nanocrystalline SZ as catalyst in high yields. ► Compared to previously reported methods, Moreover, the mild reaction conditions, easy work-up, clean reaction profiles, lower catalyst loading and cost efficiency render this approach as an interesting alternative to the existing methods. The catalysts can be recovered for the subsequent reactions and reused without any appreciable loss of their efficiency.

 $\triangleright$  CH<sub>4</sub> conversion to C<sub>2</sub> + correlates with the number of basic sites of oxide catalysts.  $\triangleright$  C<sub>2</sub> + is formed only



#### Florica Papa, Patron Luminita, Petre Osiceanu, Ruxandra Birjega, Miyazaki Akane, Ioan Balint

Journal of Molecular Catalysis A: Chemical 346 (2011) 48

Acid-base properties of the active sites responsible for  $C_2^+$  and  $CO_2$  formation over MO–Sm<sub>2</sub>O<sub>3</sub> (M = Zn, Mg, Ca and Sr) mixed oxides in OCM reaction

when surface carbonate decomposes to generate free basic sites. ► The amount of available basic sites can calculated from the amount of desorbed  $CO_2$ .  $\blacktriangleright$  CH<sub>4</sub> is unselectively oxidized to CO<sub>2</sub> on the acid sites of oxide catalysts. ► The activity of acid sites for CH<sub>4</sub> combustion is hindered by basic molecules (NH3).



#### Dong-Bo Cao, Yong-Wang Li, Jianguo Wang, Haijun Jiao

Journal of Molecular Catalysis A: Chemical 346 (2011) 57

Chain growth mechanism of Fischer-Tropsch synthesis on  $Fe_5C_2(0\ 0\ 1)$ 

► The chain growth mechanisms of Fischer–Tropsch synthesis on  $\text{Fe}_5C_2(0 \ 0 \ 1)$  were reported.  $\blacktriangleright$  Chain initiation from CO insertion obeys insertion mechanism. 
Chain propagation from CCH coupling obeys carbide mechanism. ► Both mechanisms are operative and co-operative in Fischer-Tropsch synthesis.

chain growth CO insertion + carbide coupling



#### Martin J. Hanton, Sergey Tin, Brian J. Boardman, Philip Miller

► The synthesis of a new tripodal phosphine ligand, N(CH<sub>2</sub>PEt<sub>2</sub>)<sub>3</sub>, NTriPhos<sup>Et</sup>. ► Ru-catalysed ester hydrogenation using the tripodal ligands N(CH2PR2)3 (R = Ph,Et). ► The effect of additives on Ru-TriPhos<sup>Ph</sup>-based ester hydrogenation. ► The kinetics of ester hydrogenation with Ru and tripodal phosphines. ► Contrasting ester hydrogenation with TriPhos<sup>Ph</sup> and N-TriPhos<sup>Ph</sup>.

Journal of Molecular Catalysis A: Chemical 346 (2011) 72

Ruthenium-catalysed hydrogenation of esters using tripodal phosphine ligands



#### Yasuhiro Yamada, Masaki Segawa, Fumiya Sato, Takashi Kojima, Satoshi Sato

Journal of Molecular Catalysis A: Chemical 346 (2011) 81

Catalytic performance of rare earth oxides in ketonization of acetic acid

► La<sub>2</sub>O<sub>3</sub>, CeO<sub>2</sub>,  $Pr_6O_{11}$ , and  $Nd_2O_3$  are active in acetone formation from acetic acid. ► During the induction period, oxyacetate is formed in La<sub>2</sub>O<sub>3</sub>,  $Pr_6O_{11}$ , and  $Nd_2O_3$ . ► Bulk structure of CeO<sub>2</sub> was stable during the ketonization. ► The catalytic ketonization proceeds over the surface of the oxyacetate and CeO<sub>2</sub>. ► Catalytic cycle is composed of two steps: decomposition and regeneration of surface acetates.



#### Manickam Sasidharan, Asim Bhaumik

Journal of Molecular Catalysis A: Chemical 346 (2011) 89

Titanium silicates as efficient catalyst for alkylation and acylation of silyl enol ethers under liquid-phase conditions Titanium silicates as efficient catalyst for alkylation and acylation of silyl enol ethers under liquid-phase conditions.  $\blacktriangleright$  Catalytic alkylation and acylation over TS-1, TS-2, Ti- $\beta$  and Sn-MFI.  $\blacktriangleright$  Alkylation and acetylation of Silyl enol ethers.  $\blacktriangleright$  Lewis acidity of titanium silicates.  $\blacktriangleright$  -Alkylation/acylation of ketones over titanium silicates.



#### Ard C.J. Koeken, Leo J.P. van den Broeke, Nieck E. Benes, Jos T.F. Keurentjes

Journal of Molecular Catalysis A: Chemical 346 (2011) 96

Triphenylphosphine modified rhodium catalyst for hydroformylation in supercritical carbon dioxide



► Evaluation of kinetics of 1-octene hydroformylation in supercritical CO<sub>2</sub>. ► The reaction is first order in

1-octene and negative order in CO and phosphine. 
Increasing phosphine ligand amount improves



#### Andreia Valente, Philippe Zinck, André Mortreux, Marc Visseaux, Paulo J.G. Mendes, Tiago J.L. Silva, M. Helena Garcia

Journal of Molecular Catalysis A: Chemical 346 (2011) 104

Polymerization of ε-caprolactone using ruthenium(II) mixed metallocene catalysts and isopropyl alcohol: Living character and mechanistic study

▶ First Ru(II) mixed metallocene catalysts for living Activated Monomer mechanism. ▶ Innovative polymerization mechanism based on arene  $\eta^6 - \eta^4$  slippage.  $\blacktriangleright$  DFT studies performed for the first time for a ROP via Activated Monomer mechanism. ► Recovery of the ruthenium catalytic complexes at the end of reaction. ► Growing of several polymer chains per metal: catalyst economy for green chemistry.

▶ A  $CoFe_2O_4$ - $Cr_2O_3$ - $SiO_2$  fluorescent magnetic nanocomposite with high band gap energy. ► The

nanocomposite acts as an efficient photocatalyst for degradation of methylene blue. ► Magnetic

nanocomposite could be recovered using an external magnet and reused.



#### Kula Kamal Senapati, Chandan Borgohain, Kanak C. Sarma, Prodeep Phukan

Journal of Molecular Catalysis A: Chemical 346 (2011) 113

Photocatalytic degradation of methylene blue in water using CoFe<sub>2</sub>O<sub>4</sub>-Cr<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> fluorescent magnetic nanocomposite







Final MB + CoFe<sub>2</sub>O<sub>4</sub>-Cr<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> Spectrum