



## Contents

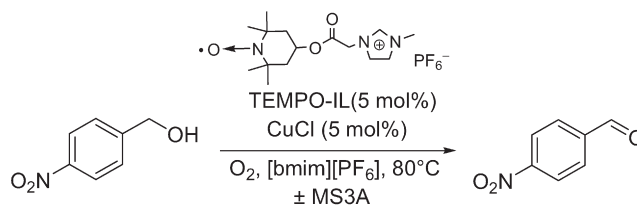
### Articles

**Liu Lin, Ma Juanjuan, Ji Liuyan, Wei Yunyang**

*Journal of Molecular Catalysis A: Chemical 291 (2008) 1*

Molecular sieve promoted copper catalyzed aerobic oxidation of alcohols to corresponding aldehydes or ketones

An efficient and selective aerobic oxidation procedure of alcohols to the corresponding aldehydes or ketones using CuCl/TEMPO-IL/MS3A catalytic system in ionic liquid [bmim][PF<sub>6</sub>] has been developed. MS3A serves as a heterogeneous Brønsted base to enhance the reaction rate remarkably. It is noteworthy to mention that the catalysts and solvent could easily be recycled and reused without loss of activity.



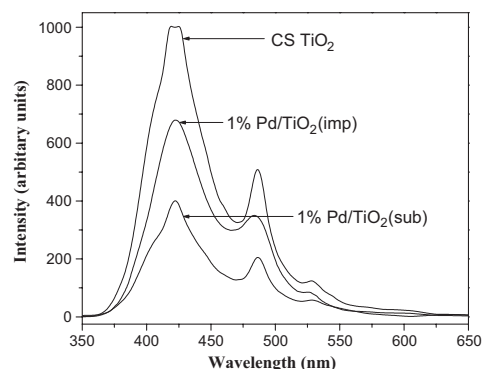
without MS3A 16 h, 98% conversion  
with MS3A 3 h, 99% conversion

**R. Vinu, Giridhar Madras**

*Journal of Molecular Catalysis A: Chemical 291 (2008) 5*

Synthesis and photoactivity of Pd substituted nano-TiO<sub>2</sub>

Palladium was substituted and impregnated on nanocrystalline anatase titania and characterized. The photocatalytic degradation of various dyes and organics was investigated under UV exposure. The degradation rate was lesser in Pd substituted and impregnated titania compared to that of unsubstituted titania and this was attributed to a decrease in photoluminescence intensity.

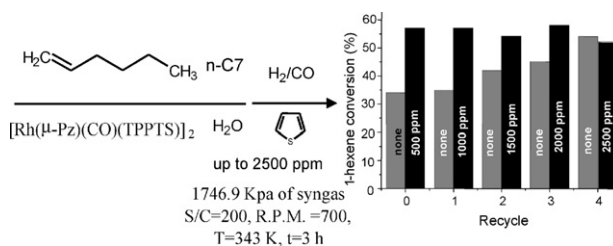


**Pablo J. Baricelli, Francisco López-Linares, Sheyla Rivera, Luis G. Melean, Victor Guanipa, Patrik Rodriguez, Mariandry Rodriguez, Merlin Rosales**

*Journal of Molecular Catalysis A: Chemical 291 (2008) 12*

Influence of the addition of thiophenes on the catalytic activity of the rhodium binuclear complex [Rh(CO)(μ-p2-Pz)(TPPTS)]<sub>2</sub> during the biphasic hydroformylation of 1-hexene

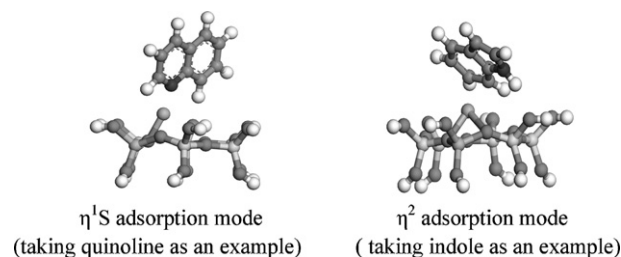
The preactivation of the binuclear complex [Rh(CO)(μ-Pz)(TPPTS)]<sub>2</sub>, TPPTS = tris-*meta*-sulfonatophenylphosphine and Pz = pyrazolate ligand, during the two-phase catalytic hydroformylation of 1-hexene was studied under mild reaction conditions [1746.9 kPa of syngas (CO/H<sub>2</sub> = 1:1), S/C = 200, R.P.M. = 700, T = 343 K, t = 3 h]. It was confirmed the formation of mononuclear active species responsible of the olefin hydroformylation. The presence of compounds such as thiophene and benzothiophene up to 2500 ppm did not interfere with the evolution of the reaction, confirming that the active specie is resistant to sulphur. It was found that under *anaerobic conditions*, the catalytic activity remains almost constant after four consecutive recycles, leading to the production of aldehydes and the corresponding isomerization products, *cis*- and *trans*-2-hexene.



**Dan Liu, Jianzhou Gui, Zhaolin Sun***Journal of Molecular Catalysis A: Chemical* 291 (2008) 17

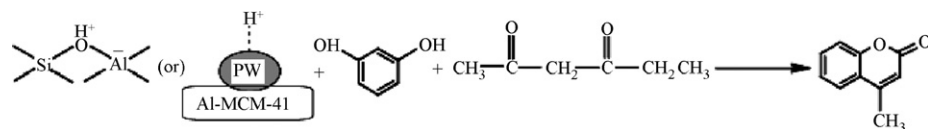
Adsorption structures of heterocyclic nitrogen compounds over Cu(I)Y zeolite: A first principle study on mechanism of the denitrogenation and the effect of nitrogen compounds on adsorptive desulfurization

The adsorption configurations of quinoline, acridine, indole and carbazole over Cu(I)Y zeolite were studied by the density functional theory (DFT) method. The  $\eta^2$  adsorption mode has been found to be energetically preferred for neutral nitrogen compounds, while for basic ones the  $\eta^1$ N adsorption mode is the most preferential one, implying that in the competitive adsorption aromatics show a strong preference over neutral nitrogen compounds than over basic ones. The adsorption energies of the adsorbate over Cu(I)Y zeolite decrease as follows: basic heterocyclic nitrogen compounds > neutral heterocyclic nitrogen compounds > thiophenic compounds, suggesting that deep denitrogenation and desulfurization could be carried out simultaneously over Cu(I)Y zeolite under ambient temperature, while Cu(I)Y zeolite is a preferable adsorbent for nitrogen compounds rather than for sulfur compounds.

**S. Sudha, K. Venkatachalam, S. Vishnu Priya, J. Herbert Mabel, M. Palanichamy, V. Murugesan***Journal of Molecular Catalysis A: Chemical* 291 (2008) 22

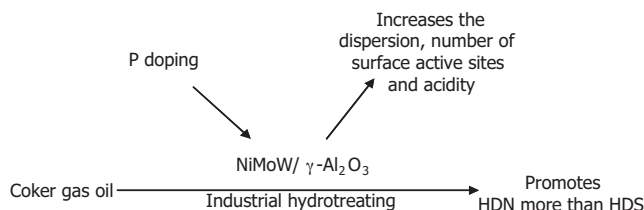
Single step synthesis of coumarin derivatives over Al-MCM-41 and its supported catalysts under solvent-free condition

Pechmann reaction has been extensively used for the preparation of coumarin and its derivatives from simple starting materials. The present investigation describes an ecofriendly route for the Pechmann synthesis of coumarin derivatives over Al-MCM-41 and its supported catalysts under solvent-free condition.

**S. Sigurdson, V. Sundaramurthy, A.K. Dalai, J. Adjaye***Journal of Molecular Catalysis A: Chemical* 291 (2008) 30

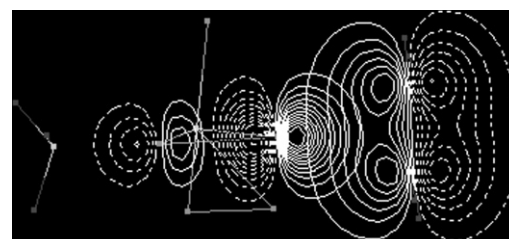
Phosphorus promoted trimetallic NiMoW/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> sulfide catalysts in gas oil hydrotreating

P doping promoted the hydrotreating activity of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>-supported NiMoW trimetallic catalyst. P promoted NiMoW/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> sulfide catalyst with 1.6 wt.% P, 6.9 wt.% W, 5.2 wt.% Mo and 2.4 wt.% of Ni showed superior hydrotreating activity than the P-doped bimetallic NiMo, NiW and commercial catalysts with gas oil derived from Athabasca bitumen at industrial conditions.

**Akinobu Shiga, Yasuhiko Kurusu***Journal of Molecular Catalysis A: Chemical* 291 (2008) 38

Theoretical study on selective oxidation of olefin and alcohol with Mo-peroxo amine complex using "paired interacting orbitals (PIOs)" analysis

Oxidation mechanisms of ethylene and methanol on Mo(O)(OO)<sub>2</sub> (an amine) are studied. In the case of ethylene oxidation PIO analysis reveals that the electron delocalization from the  $\sigma^*$ -orbital of the ethylene to the  $\sigma^*$ -orbital (O<sup>3</sup>-O<sup>4</sup>) of the Mo peroxo (the so called  $\pi$ -donation of ethylene), the electron delocalization from the p-orbital of O<sup>4</sup> of the Mo peroxo to the  $\pi^*$ -orbital of the ethylene and the overlap repulsion between occupied orbitals of the ethylene and occupied (Mo-O<sup>3</sup>-O<sup>4</sup>) orbitals of the Mo peroxo. This overlap repulsion is enhanced by the coordination of higher alkyl amines to the Mo peroxo, because of the destabilization of these occupied (Mo-O<sup>3</sup>-O<sup>4</sup>) orbitals. So, the results suggest that ethylene epoxidation is hindered by the coordination of higher alkyl amines. On the contrary, in the case of methanol oxidation, methanol coordination to the Mo peroxo moiety, Mo-methoxy complex formation and hydrogen abstraction which are elementary reactions of methanol oxidation, are not hindered by the coordination of amines. This is one reason why a selective oxidation of alcohols is attained by addition of higher alkyl amines to the oxidation system.



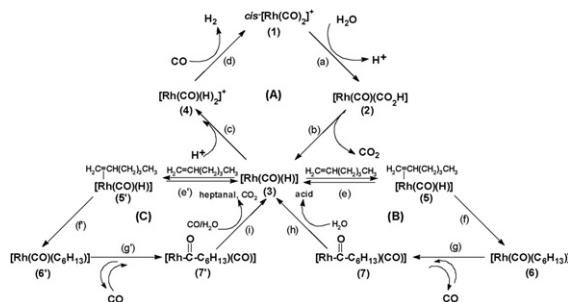
Contour maps of PIO-1 of model (2)

**Germán Gascón, Marisol C. Ortega,  
José D. Suárez Alvaro J. Pardey,  
Clementina Longo, Sergio A. Moya**

*Journal of Molecular Catalysis A: Chemical* 291 (2008) 49

Carbonylation of 1-hexene catalyzed by *cis*-[Rh(CO)<sub>2</sub>(amine)<sub>2</sub>](PF<sub>6</sub>) complexes in aqueous tetrabutylammonium hydrogensulfate solutions

In this work, carbonylation of 1-hexene to heptanoic acid and heptanal catalyzed by rhodium(I) complexes, *cis*-[Rh(CO)<sub>2</sub>(amine)<sub>2</sub>](PF<sub>6</sub>) (amine = pyridine, 2-picoline, 3-picoline, 4-picoline, 3,5-lutidine or 2,6-lutidine) dissolved in aqueous solution of tetrabutylammonium hydrogensulfate (N(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>HSO<sub>4</sub>), under carbon monoxide atmosphere, is described. Gaseous by-products (H<sub>2</sub> and CO<sub>2</sub>) from the catalysis of the water–gas shift reaction (WGSR) were also produced. The reaction products distribution depends on the nature of the coordinated amine to the rhodium center. The effects of variation of CO pressure, temperature, catalyst concentration, 1-hexene/Rh molar ratio and N(C<sub>4</sub>H<sub>9</sub>)<sub>4</sub>HSO<sub>4</sub> amount, on the reaction rates were also examined.

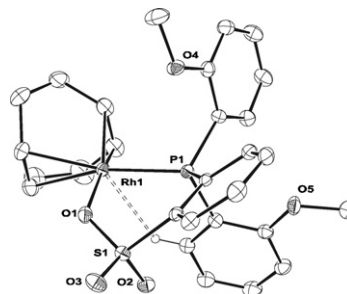


**Lorenzo Bettucci, Claudio Bianchini, Andrea Meli,  
Werner Oberhauser**

*Journal of Molecular Catalysis A: Chemical* 291 (2008) 57

Synthesis of neutral rhodium(I) complexes containing a rigid P–O ligand and their use as catalyst precursors for the hydroformylation of 1-hexene

The first rhodium(I) complexes with the anionic 2-(bis(2-methoxyphenyl)phosphino)benzenesulfonate (L) ligand have been synthesized and characterized. Selected complexes have been used as catalyst precursors for the homogeneous hydroformylation of 1-hexene.

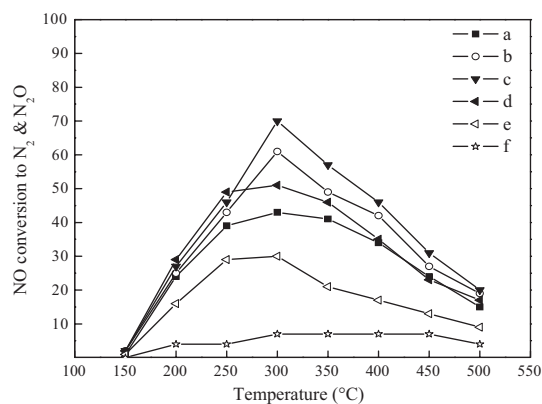


**Pullur Anil Kumar, Maddigapu Pratap Reddy,  
Lee Kyung Ju, Bae Hyun-Sook, Ha Heon Phil**

*Journal of Molecular Catalysis A: Chemical* 291 (2008) 66

Low temperature propylene SCR of NO by copper alumina catalyst

A high conversion (70%) of NO to N<sub>2</sub> was obtained by the Cu–Al (3:7) catalyst at 300 °C in the presence of 600 ppm NO<sub>x</sub> + 600 ppm C<sub>3</sub>H<sub>6</sub> + 8 vol.% O<sub>2</sub>. The order of catalysts for higher NO to N<sub>2</sub> conversion is as follows: Cu–Al (3:7) > Cu–Al (2:8) > Cu–Al (4:6) > Cu–Al (1:9) > Cu–Al (7:3). The XPS results show that the Cu–Al (3:7) catalysts calcined at 600 °C possess highly dispersed surface copper (Cu<sup>2+</sup>) species. The presence of high surface availability of copper (% intensity of 44.8) and in particular as CuAl<sub>2</sub>O<sub>4</sub> phase with a high percent intensity of 44 in the Cu–Al (3:7) catalyst is the key to obtaining high efficiency (70%) in a wide range of temperatures (250–400 °C).



**Jose Iglesias, Juan A. Melero, Javier Sainz-Pardo**

*Journal of Molecular Catalysis A: Chemical* 291 (2008) 75

Direct synthesis of organically modified Ti-SBA-15 materials

Organically functionalized titanium-containing SBA-15-type materials were prepared, following a direct synthesis procedure involving the co-condensation of all of the synthesis precursors in a single step. The hybrid organic–inorganic Ti-SBA-15 materials drive the oxidation of 1-octene with TBHP, being the intrinsic catalytic activity controlled by the size of the organic functionality because of modification of the titanium sites microenvironment.

