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## Journal of Molecular Catalysis A: Chemical

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## Contents

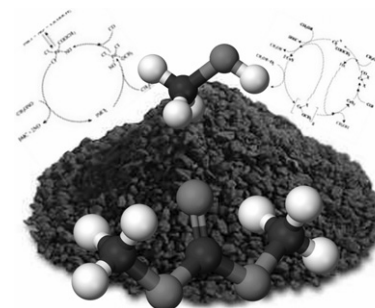
## Articles

**Nicolas Keller, Guillaume Rebmann,  
Valérie Keller**

*Journal of Molecular Catalysis A: Chemical 317 (2010) 1*

Catalysts, mechanisms and industrial processes for the dimethylcarbonate synthesis

This review deals with the chemical uses and synthesis ways of dimethylcarbonate (DMC) with special focus on the vapour phase oxycarbonylation of methanol by carbon monoxide, and highlights both chlore-containing and chlore-free active catalysts, their reaction mechanisms as well as the industrial processes and the reactions for producing DMC.

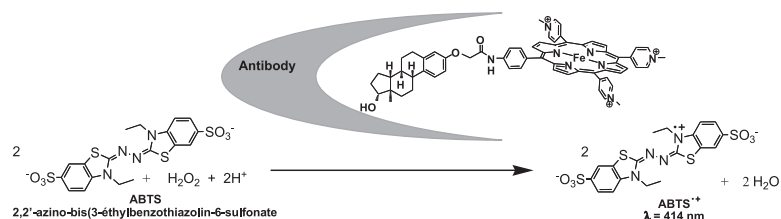


**Quentin Raffy, Rémy Ricoux, Elodie Sansiaume,  
Stéphanie Pethe, Jean-Pierre Mahy**

*Journal of Molecular Catalysis A: Chemical 317 (2010) 19*

Coordination chemistry studies and peroxidase activity of a new artificial metalloenzyme built by the “Trojan horse” strategy

The association of an anti-estradiol antibody with an iron–porphyrin–estradiol cofactor by the “Trojan horse” strategy leads to a new artificial hemoprotein with an interesting peroxidase activity that catalyzes the oxidation of ABTS by  $\text{H}_2\text{O}_2$  twice faster than the cofactor alone. This is due to a twice faster formation of the intermediate iron–oxo species in the presence of the antibody.

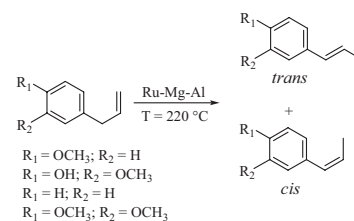


**Sumeet K. Sharma, Parimal A. Parikh,  
Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical 317 (2010) 27*

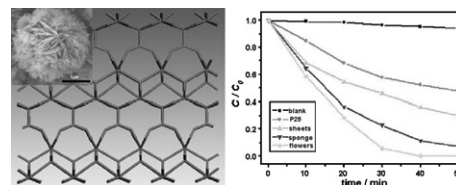
Ruthenium containing hydrotalcite as a solid base catalyst for  $>\text{C}=\text{C}<$  double bond isomerization in perfumery chemicals

Ruthenium containing hydrotalcite (Ru–Mg–Al) is reported as a solid base catalyst for double bond isomerization of methyl chavicol, eugenol, safrole, allylbenzene, dimethoxy allylbenzene and 3-carene. The activity of Ru–Mg–Al was compared with the various ruthenium impregnated catalysts such as, Ru–HT, Ru–MgO, Ru–CaO, Ru– $\text{SiO}_2$  and Ru–alumina.



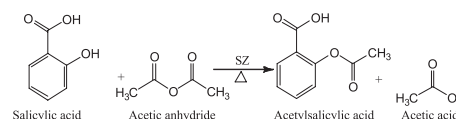
**Yan Zheng, Fang Duan, Mingqing Chen, Yi Xie***Journal of Molecular Catalysis A: Chemical* 317 (2010) 34Synthetic  $\text{Bi}_2\text{O}_2\text{CO}_3$  nanostructures: Novel photocatalyst with controlled special surface exposed

A series of novel  $\text{Bi}_2\text{O}_2\text{CO}_3$  photocatalysts was first put forward by virtue of structural understanding. The flower-like  $\text{Bi}_2\text{O}_2\text{CO}_3$  hierarchitecture with the controlled special  $\{001\}$  surface exposed was first synthesized via a mild route, showing the excellent photocatalytic activity under the solar light due to the large distortion of Bi–O on the exposed surface.

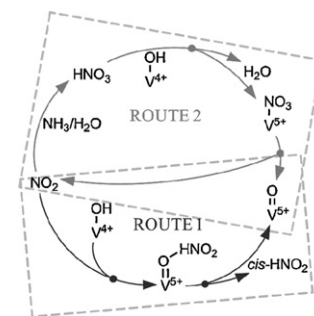
**Beena Tyagi, Manish Kumar Mishra, Raksh Vir Jasra***Journal of Molecular Catalysis A: Chemical* 317 (2010) 41

Solvent free synthesis of acetyl salicylic acid over nano-crystalline sulfated zirconia solid acid catalyst

An eco-friendly, solvent free synthesis of acetyl salicylic acid has been carried out over various solid acid catalysts. Among all the catalysts studied nano-crystalline sulfated zirconia (SZ) catalyst showed highest catalytic activity yielding 95 wt% of acetyl salicylic acid. Thermally regenerated catalyst showed similar yield as obtained with the fresh catalyst.

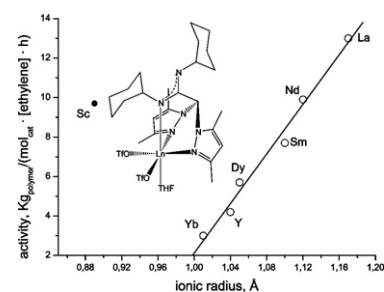
**Xiang Gao, Xue-sen Du, Ye Jiang, Yang Zhang, Zhong-yang Luo, Ke-fa Cen***Journal of Molecular Catalysis A: Chemical* 317 (2010) 46A DFT study on the behavior of  $\text{NO}_2$  in the selective catalytic reduction of nitric oxides with ammonia on a  $\text{V}_2\text{O}_5$  catalyst surface

DFT calculations were carried out to study the behavior of  $\text{NO}_2$  in the selective catalytic reduction (SCR) of nitric oxides with ammonia on the surface of the  $\text{V}_2\text{O}_5$  catalyst. A systematic description of the behavior for  $\text{NO}_2$  in "fast" SCR on the  $\text{V}_2\text{O}_5$  surface, including the reaction routes and energy profiles, is proposed in this work.

**Gino Paolucci, Marco Bortoluzzi, Mariagrazia Napoli, Pasquale Longo, Valerio Bertolasi***Journal of Molecular Catalysis A: Chemical* 317 (2010) 54

The role of the ionic radius in the ethylene polymerization catalyzed by new group 3 and lanthanide scorpionate complexes

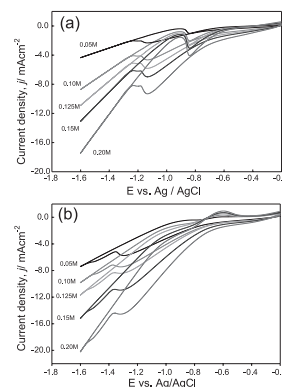
New group 3 and lanthanide [N,N,N]-heteroscorpionate triflate-complexes  $[\text{Ln}(\text{OTf})_2(\text{cybpamd})(\text{THF})]$  have been synthesized. The behavior as polymerization catalysts was investigated and the comparative results are reported.



M.A. Hasnat, M. Amirul Islam, S.M. Borhanuddin,  
M.R. Ullah Chowdhury, M. Machida

*Journal of Molecular Catalysis A: Chemical* 317 (2010) 61

Influence of Rh on electrocatalytic reduction of  $\text{NO}_3^-$   
and  $\text{NO}_2^-$  over Pt and Pd films

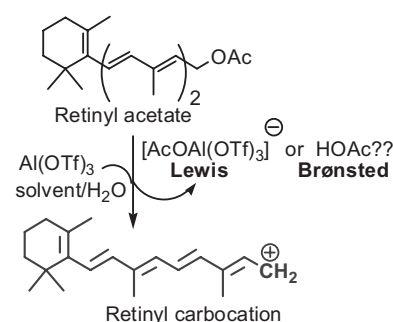


D. Bradley G. Williams, Michelle Lawton

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Metal triflates: On the question of Lewis versus  
Brønsted acidity in retinyl carbocation formation

Retinyl acetate liberates intense blue carbocations with Brønsted acids.  $\text{Al}(\text{OTf})_3$  also generates such carbocations apparently exclusively via water-derived induced Brønsted acidity (loss of acetic acid) as opposed to the Lewis acid acting as an acetate abstractor.

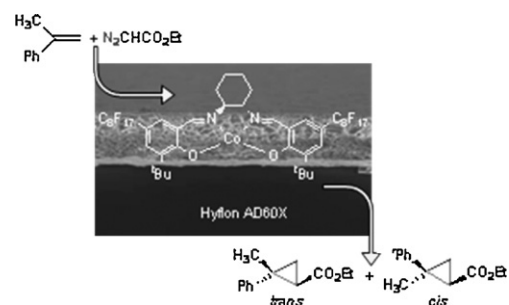


Alessandro Caselli, Maria Giovanna Buonomenna,  
Federico de Baldironi, Luca Laera, Simone Fantauzzi,  
Fabio Ragaini, Emma Gallo, Giovanni Golemme,  
Sergio Cenini, Enrico Drioli

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From homogeneously to heterogeneously catalyzed  
cyclopropanation reactions: New polymeric membranes  
embedding cobalt chiral schiff base complexes

The new catalytic membranes having the complex  $[(N,N'\text{-bis}(3\text{-tert-butyl-5-(heptadecafluorooctyl)salicylidene)-trans\text{-}1,2\text{-cyclohexanediamine})\text{Co}]$  embedded into Hyflon AD60X, PES and PSf have been prepared and characterized and their use in the cyclopropanation reaction of olefins with ethyl diazoacetate (EDA) is reported.

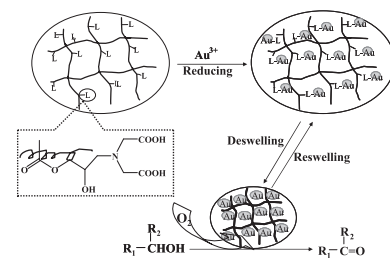


Yao Wang, Rui Yan, Jianzheng Zhang,  
Wangqing Zhang

*Journal of Molecular Catalysis A: Chemical* 317 (2010) 81

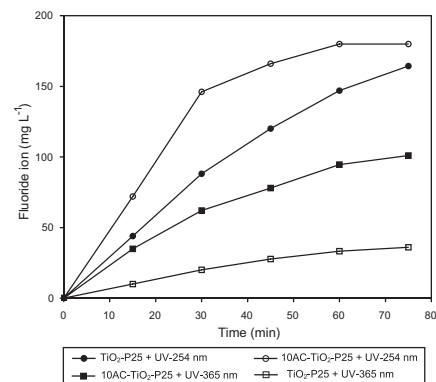
Synthesis of efficient and reusable catalyst of size-  
controlled Au nanoparticles within a porous,  
chelating and intelligent hydrogel for aerobic alcohol  
oxidation

Synthesis of size-controlled Au nanoparticles within a porous, chelating and intelligent hydrogel is achieved. The resultant hydrogel/Au composite is thermoresponsive, which can reversibly deswell/swell at the volume-phase-transition temperature. Alcohol and Au nanocatalyst can be highly concentrated within the hydrogel matrix by the reversible deswelling/swelling of the thermoresponsive composite and therefore aerobic alcohol oxidation runs efficiently.



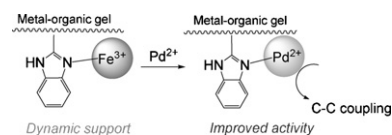
**L. Ravichandran, K. Selvam, M. Swaminathan***Journal of Molecular Catalysis A: Chemical* 317 (2010) 89Highly efficient activated carbon loaded TiO<sub>2</sub> for photo defluorination of pentafluorobenzoic acid

Defluorination is more effective in 10AC-TiO<sub>2</sub>-P25 than bare TiO<sub>2</sub>-P25 and 254 nm is more effective than 365 nm. The higher efficiency of AC-TiO<sub>2</sub>-P25 is due to synergy effect of activated carbon.

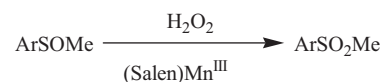
**Jing Huang, Lisi He, Jianyong Zhang, Liuping Chen, Cheng-Yong Su***Journal of Molecular Catalysis A: Chemical* 317 (2010) 97

Dynamic functionalised metallo gel: An approach to immobilised catalysis with improved activity

A metal-organic gel route to immobilised catalysts has been developed based on the reversibility of coordination bond formation in a ferric gel based on 5-1*H*-benzo[*d*]imidazole-1,3-dicarboxylic acid. Palladium(II) was efficiently loaded in the gel due to the HSAB matching. The immobilised gel exhibited significantly improved catalytic activity as shown in Suzuki-Miyaura coupling, and could be reused.

**Arunachalam Chellamani, Paramasivan Sengu, Naina Mohamed Ismail Alhaji***Journal of Molecular Catalysis A: Chemical* 317 (2010) 104Kinetics and mechanism of oxidation of aryl methyl sulfoxides with (salen)Mn<sup>III</sup>/H<sub>2</sub>O<sub>2</sub> catalytic system

The oxidation of aryl methyl sulfoxides with H<sub>2</sub>O<sub>2</sub> in the presence of (salen)Mn<sup>III</sup> complex is first-order in complex, zero-order in H<sub>2</sub>O<sub>2</sub> and fractional-order in sulfoxide. A Michaelis-Menten type mechanism involving Mn<sup>III</sup>-hydroperoxide complex as reactive species has been proposed.

**V. Udayakumar, S. Alexander, V. Gayathri Shivakumaraiah, K.R. Patil, B. Viswanathan***Journal of Molecular Catalysis A: Chemical* 317 (2010) 111

Polymer-supported palladium-imidazole complex catalyst for hydrogenation of substituted benzylideneanilines

The polymer-supported palladium-imidazole complex catalyst was synthesized, characterized and investigated for hydrogenation of benzylideneaniline and its derivatives. Kinetics studies and the effect of few substituents in the para position of benzaldehyde ring of benzylideneaniline were carried out and a plausible mechanism and rate equation have been proposed.

