

## Contents

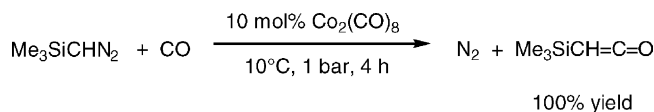
### Articles

**Neszta Ungvári, Tamás Kégl, Ferenc Ungváry**

*Journal of Molecular Catalysis A: Chemical 219 (2004) 7*

Octacarbonyl dicobalt-catalyzed selective carbonylation of (trimethylsilyl)diazomethane to obtain (trimethylsilyl)ketene

The selective carbonylation of (trimethylsilyl)diazomethane to (trimethylsilyl)ketene in the presence of octacarbonyl dicobalt is the first highly efficient catalytic reaction in which a carbene carbon monoxide coupling is involved.

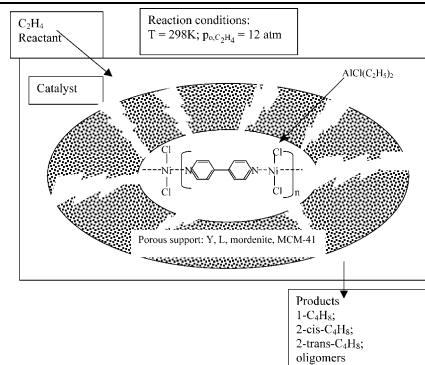


**Emilian Angelescu, Michel Che, Marius Andruh, Rodica Zăvoianu, Guylène Costentin, Cătălin Mirică, Octavian Dumitru Pavel**

*Journal of Molecular Catalysis A: Chemical 219 (2004) 13*

Ethylene selective dimerization on polymer complex catalyst of Ni(4,4'-bipyridine)Cl<sub>2</sub> coactivated with AlCl(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>

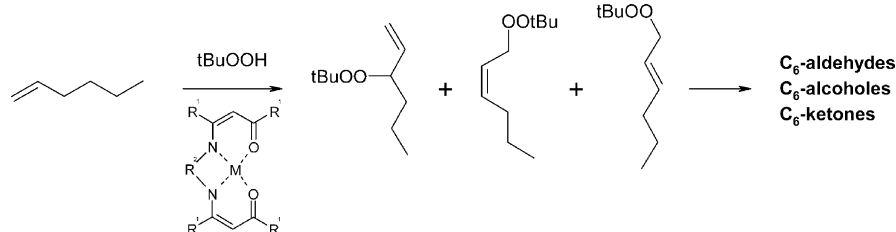
The polymer complex Ni(4,4'-bipyridine)Cl<sub>2</sub> co-activated with AlCl(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub> and dispersed on micro- or mesoporous supports is an active and selective catalyst for ethylene dimerization to normal butenes under mild reaction conditions. The complex supported on MCM-41 molecular sieve exhibited the highest activity and allowed also the obtaining of highest amounts of oligomers.



**Juha Pulkkinen, Pavel Zachar, Vojtech Albert Borek, Reino Laatikainen, Vladimir Kral**

*Journal of Molecular Catalysis A: Chemical 219 (2004) 21*

Application of novel metallocomplexes for mimicking of cytochrome P450. Analysis of product distribution for 1-hexene as a substrate

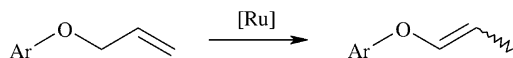


**Stanisław Krompiec, Nikodem Kuźnik,  
Robert Penczek, Józef Rzepa,  
Julita Mrowiec-Białoń**

*Journal of Molecular Catalysis A: Chemical* 219  
(2004) 29

Isomerization of allyl aryl ethers to their 1-propenyl derivatives catalysed by ruthenium complexes

Double bond migration in allyl aryl ethers was catalysed by ruthenium complexes. Interesting *E/Z* control was achieved using  $[\text{RuCl}_2(\text{COD})]_x + \text{PR}_3$  catalytic system.



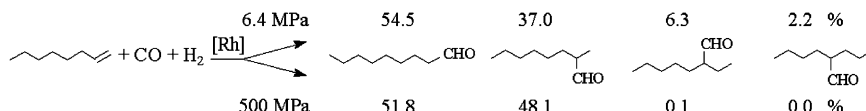
$[\text{Ru}] = [\text{RuCl}(\text{H})(\text{CO})(\text{PPh}_3)_3], [\text{RuCl}_2(1,5\text{-cod})] + \text{PR}_3, \dots$   
Ar = Ph, Cl-C<sub>6</sub>H<sub>4</sub>, O<sub>2</sub>N-C<sub>6</sub>H<sub>4</sub>, OHC-C<sub>6</sub>H<sub>4</sub>, AllilO-C<sub>6</sub>H<sub>4</sub>, ...

**Jörn Albers, Eckhard Dinjus, Stephan Pitter,  
Olaf Walter**

*Journal of Molecular Catalysis A: Chemical* 219  
(2004) 41

High-pressure effects in the homogeneously catalyzed hydroformylation of olefins

The homogeneously catalyzed hydroformylation of linear olefins was investigated at pressures ranging from 7 to 550 MPa. A change in the selectivity was observed, which was reflected by a change of the product distribution. At high pressures, increased yields of aldehydes were also obtained from the hydroformylation of sterically hindered olefins.



**L. Bonoldi, L. Abis, L. Fiocca, R. Fusco,  
L. Longo, F. Simone, S. Spera**

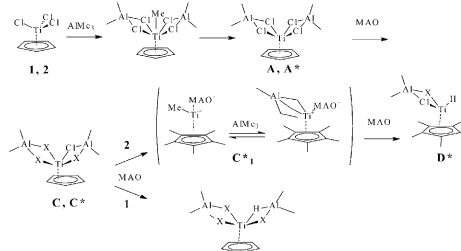
*Journal of Molecular Catalysis A: Chemical* 219  
(2004) 47

Monotitanocene catalysts: an ESR study of Ti(III) derivatives formed in presence of MAO and other organoaluminium compounds

The Ti(III) complexes generated in the reaction of  $\text{Cp}'\text{TiCl}_3$  [ $\text{Cp}' = \text{C}_5\text{H}_5 = \text{Cp}$  (**1**),  $\text{C}_5\text{Me}_5 = \text{Cp}^*$  (**2**),  $\text{Me} = \text{CH}_3$ ] with methyl-aluminoxane (MAO) were investigated by the electron spin resonance (ESR) technique.

At low Al/Ti molar ratio (10) the only product is the trinuclear bimetallic complex  $\text{Cp}'\text{Ti}[(\mu\text{-Cl})_2\text{AlMe}_2]_2$  (**A**, **A**<sup>\*</sup>).

At higher Al/Ti ratio (300, 500) a stable titanium hydride compound (**D**) forms in the system **1**/MAO while in the system **2**/MAO two alkylated species appear, one of which is the cationic one  $[\text{Cp}'\text{TiMe}]^{+\ast}\text{AlMe}_3$ .

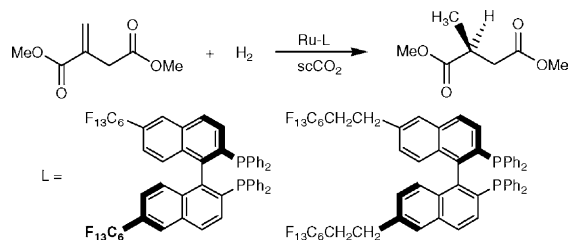


**Yulai Hu, David J. Birdsall, Alison M. Stuart,  
Eric G. Hope, Jianliang Xiao**

*Journal of Molecular Catalysis A: Chemical* 219  
(2004) 57

Ruthenium-catalysed asymmetric hydrogenation with fluoroalkylated BINAP ligands in supercritical CO<sub>2</sub>

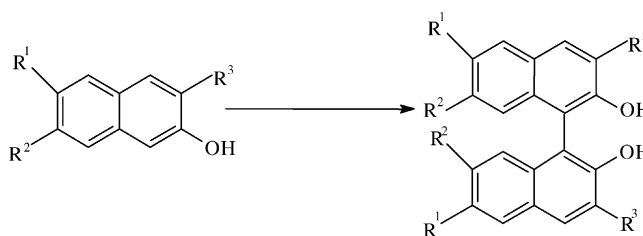
Fluoroalkylated BINAP ligands have been evaluated in the ruthenium-catalysed asymmetric hydrogenation of dimethyl itaconate in supercritical CO<sub>2</sub> as well as MeOH.



**Vishal B. Sharma, Suman L. Jain, Bir Sain**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 61

Copper (II) Schiff base catalysed aerobic oxidative coupling of 2-naphthols: an efficient and simple synthesis of binaphthols

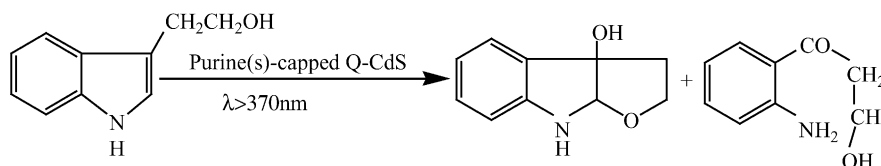


**Anil Kumar, Shipra Mital**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 65

Electronic and photocatalytic properties of purine(s)-capped CdS nanoparticles in the presence of tryptophol

Tryptophol replaces the loosely bound purine from the outer shell of the purine(s)-capped Q-CdS. Visible light irradiation of the oxygenated reaction mixture containing purine(s)-capped Q-CdS and tryptophol yields 3-hydroxyindoline and 1-(2-aminophenyl)-3-hydroxypropan-1-one as the products of oxidation. Dynamics of charge carriers and their reactivity in the irradiated CdS differ for different purine(s) used as capping agent.

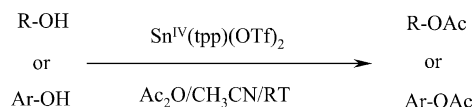


**Majid Moghadam, Shahram Tangestaninejad, Valiollah Mirkhani, Iraj Mohammadpour-Baltork, Reza Shaibani**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 73

Rapid and efficient acetylation of alcohols and phenols with acetic anhydride catalyzed by electron-deficient tin(IV) porphyrin

Rapid and efficient esterification of primary, sterically-hindered secondary and tertiary alcohols, and phenols with acetic anhydride: was achieved in the presence of  $\text{Sn}^{\text{IV}}(\text{tpp})(\text{CF}_3\text{SO}_3)_2$  as catalyst in high yields.

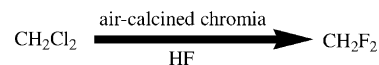


**Heng-dao Quan, Masanori Tamura, Yasuhisa Matsukawa, Junji Mizukado, Takashi Abe, Akira Sekiya**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 79

Investigation into chromia-based catalyst and its application in preparing difluoromethane

A high oxidation state of Cr species exists in the air-calcined chromia-based catalysts, which exhibit a higher catalytic activity than Cr(III). Moreover, the treatment of chromia with HF at low temperature leads to facile crystallization of the chromia-based catalyst and a decrease in the catalytic activity.

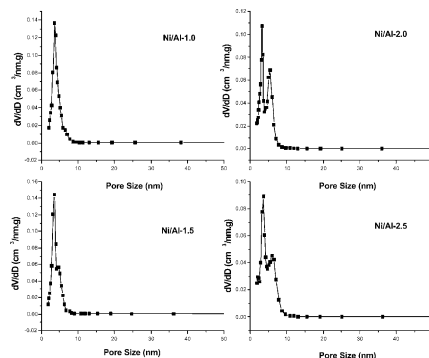


**Pil Kim, Younghun Kim, Heesoo Kim,  
In Kyu Song, Jongheop Yi**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 87

Synthesis and characterization of mesoporous alumina for use as a catalyst support in the hydrodechlorination of 1,2-dichloropropane: effect of preparation condition of mesoporous alumina

Mesoporous  $\gamma$ -aluminas were synthesized by a post-hydrolysis method with different mole ratios of surfactant/aluminum precursor. The effect of mole ratio of surfactant/aluminum precursor on the catalytic performance of Ni/ $\gamma$ -alumina catalysts was investigated for the hydrodechlorination of 1,2-dichloropropane (DCPA).

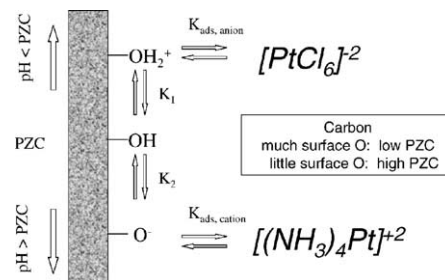


**X. Hao, L. Quach, J. Korah, W.A. Spieker,  
John R. Regalbuto**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 97

The control of platinum impregnation by PZC alteration of oxides and carbon

While ion-doped oxides do not follow the electrostatic adsorption mechanism shown below, the adsorptive properties of carbon can be controlled by varying the carbon point of zero charge (PZC).

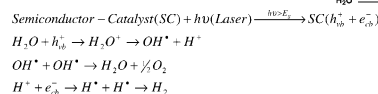
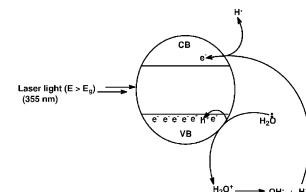


**A. Hameed, M.A. Gondal**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 109

Laser induced photocatalytic generation of hydrogen and oxygen over NiO and TiO₂

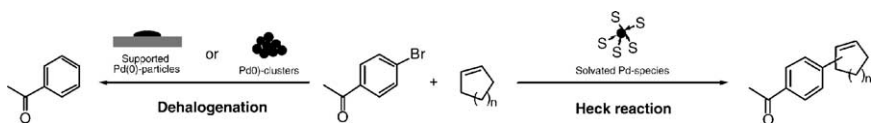
A comparative study of photocatalytic splitting of water into hydrogen and oxygen over NiO and TiO₂ was carried out using 355 nm laser radiations. It was observed that by using a monochromatic high photon flux light source, such as laser, the problem of low photonic efficiencies could be resolved.



**L. Djakovitch, M. Wagner, C.G. Hartung,  
M. Beller, K. Koehler**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 121

Pd-catalyzed Heck arylation of cycloalkenes—studies on selectivity comparing homogeneous and heterogeneous catalysts

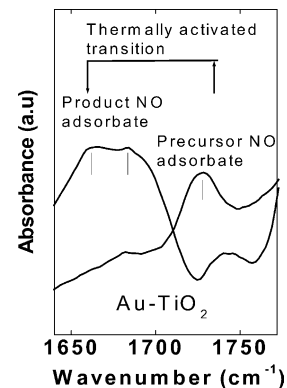


**M.A. Debeila, N.J. Coville, M.S. Scurrall, G.R. Hearne**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 131

Direct observation of thermally activated NO adsorbate species on Au-TiO<sub>2</sub>: DRIFTS studies

No adsorbate (precursor) state, detected at room temperature, changed to the product state under thermal activation. The product state is thermally stable and once is formed, is irreversible.

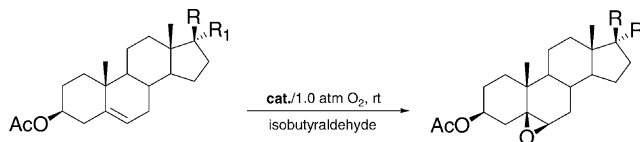


**Samuel M. Silvestre, Jorge A.R. Salvador, James H. Clark**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 143

$\beta$ -Selective epoxidation of  $\Delta^5$ -steroids by O<sub>2</sub> using surface functionalised silica supported cobalt catalysts

A general catalytic and relatively environment friendly method for  $\beta$ -epoxidation of  $\Delta^5$ -steroids has been developed, which uses silica supported cobalt as catalysts and molecular oxygen as the oxidant. The reactions are regio- and stereoselective.

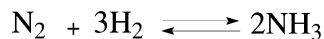


**S.M. Yunusov, E.S. Kalyuzhnaya, B.L. Moroz, A.S. Ivanova, T.V. Reshetenko, L.B. Avdeeva, V.A. Likhonobov, V.B. Shur**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 149

New ammonia synthesis catalysts based on supported potassium carbonyl ruthenates as precursors of catalytically active ruthenium particles and potassium promoter

New supported "single-component" ruthenium catalysts for ammonia synthesis derived from various potassium carbonyl ruthenates such as K<sub>2</sub>[Ru<sub>6</sub>(CO)<sub>18</sub>], K<sub>4</sub>[Ru<sub>4</sub>(CO)<sub>12</sub>], K<sub>6</sub>[Ru<sub>6</sub>(CO)<sub>16</sub>], K<sub>6</sub>[Ru<sub>4</sub>(CO)<sub>11</sub>] and K<sub>2</sub>[Ru(CO)<sub>4</sub>] are reported. The highest activity is exhibited by the K<sub>6</sub>[Ru<sub>4</sub>(CO)<sub>11</sub>]- and K<sub>2</sub>[Ru(CO)<sub>4</sub>]-based systems. An introduction of potassium metal into the catalysts leads to further increase in the ammonia synthesis rate.



250-400°C, 1 atm, Ru/support = 9 wt. %

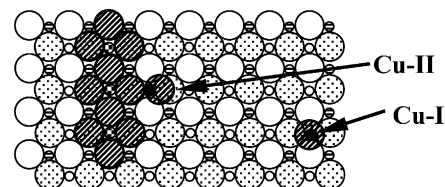
Supports: "Sibunit" and CFC-III carbons, MgO,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>/C

**Haiyang Zhu, Mingmin Shen, Yan Kong, Jianming Hong, Yuhai Hu, Tiandong Liu, Lin Dong, Yi Chen, Can Jian, Zhong Liu**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 155

Characterization of copper oxide supported on ceria-modified anatase

The dispersion of copper oxide and the state of the dispersed copper oxide species on ceria-modified TiO<sub>2</sub> closely depend on the ceria loading amounts.

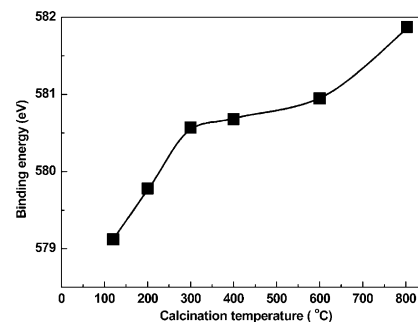


**Boping Liu, Yuwei Fang, Minoru Terano**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 165

High resolution X-ray photoelectron spectroscopic analysis of transformation of surface chromium species on Phillips  $\text{CrO}_x/\text{SiO}_2$  catalysts isothermally calcined at various temperatures

The specific transformation of Cr(III) acetate into bulky  $\text{CrO}_3$  and subsequently into chromate species ( $\text{Cr(VI)O}_{x,\text{surf}}$ ) on Phillips catalysts isothermally calcined at various temperatures (120 ~ 800 °C) has been elucidated by XPS. As the precursor of active site on calcined Phillips catalyst, chromate species was found to be gradually becoming more electron-deficient with increasing calcination temperature of the catalyst.

**Qingrong Peng, Yong Yang, Youzhu Yuan**

*Journal of Molecular Catalysis A: Chemical* 219 (2004) 175

Immobilization of rhodium complexes ligated with triphenylphosphine analogs on amino-functionalized MCM-41 and MCM-48 for 1-hexene hydroformylation

The Rh–P complexes attached to amino-group functionalized MCM-41 and MCM-48 showed catalytic activity and normal heptanal selectivity comparable to the corresponding homogeneous ones for the hydroformylation of 1-hexene. The advantage in the product selectivity towards the normal heptanal due to the larger cone angle of the ligands over Rh– $\text{PPh}_3$  in the homogeneous systems was also observed in the heterogeneous ones.

