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## Journal of Molecular Catalysis A: Chemical

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## Contents

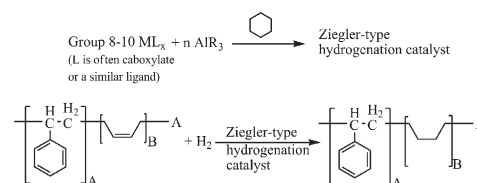
## Articles

**William M. Alley, Isil K. Hamdemir,  
Kimberly A. Johnson, Richard G. Finke**

*Journal of Molecular Catalysis A: Chemical 315 (2010) 1*

Ziegler-type hydrogenation catalysts made from group 8–10 transition metal precatalysts and  $\text{AlR}_3$  cocatalysts: A critical review of the literature

Ziegler-type hydrogenation catalysts (group 8–10 transition metal precatalysts plus  $\text{AlR}_3$  cocatalysts) are one of the most important families of industrial hydrogenation catalysts, especially for polymer hydrogenation. This review examines the existing literature on the subject of Ziegler-type hydrogenation catalysts, with an emphasis on catalyst preparation variables, if the true catalyst is homogeneous (monometallic) or heterogeneous (nanoclusters), and on approaches to the historically perplexing “it is homogeneous or heterogeneous catalysis?” question.

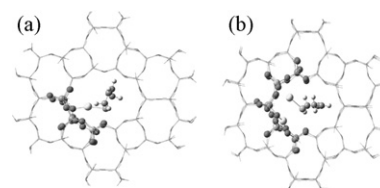


**Beulah Griffe, Joaquín L. Brito, Anibal Sierraalta**

*Journal of Molecular Catalysis A: Chemical 315 (2010) 28*

Theoretical study of Au/SAPO-11 catalyst and its potential use in thiophene HDS

Quantum chemistry calculations were carried out, using ONIOM2 methodology, in order to investigate the thiophene interaction with Au/SAPO-11 catalysts and further hydrogenation. The partial hydrogenation of the thiophene–Au/SAPO-11 complexes gives 2,5-dihydrothiophene (DHT) as seen in the figure.



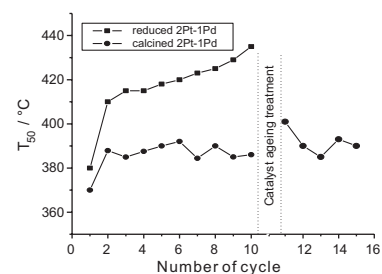
2,5- DHT obtained by hydrogenation of thiophene: a) on Au/SAPO-11; b) on Au2/SAPO-11.

**Grisel Corro, Carlos Cano, J.L.G. Fierro**

*Journal of Molecular Catalysis A: Chemical 315 (2010) 35*

A study of Pt–Pd/ $\gamma$ - $\text{Al}_2\text{O}_3$  catalysts for methane oxidation resistant to deactivation by sulfur poisoning

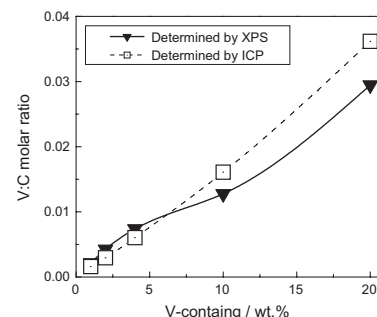
The catalytic oxidation of methane was studied over calcined, and reduced Pt–Pd/ $\gamma$ - $\text{Al}_2\text{O}_3$  catalysts, in the presence and the absence of  $\text{SO}_2$  in the  $\text{CH}_4$ – $\text{O}_2$  reaction feed. XPS analysis revealed that the presence of Pt(0) may be necessary to prevent the interactions between  $\text{SO}_2$  and Pd surface species. Long time catalytic tests showed that the activity of a reduced Pt–Pd/ $\gamma$ - $\text{Al}_2\text{O}_3$  catalysts for  $\text{CH}_4$ – $\text{O}_2$  reactions remained rather unaffected despite the presence of  $\text{SO}_2$  in the feed. Evolution of  $T_{50}$  for methane on the  $\text{CH}_4 + \text{O}_2$  reaction, with the number of temperature-programmed reaction cycles over reduced 2%Pt–1%Pd/ $\gamma$ - $\text{Al}_2\text{O}_3$ , and calcined 2%Pt–1%Pd/ $\gamma$ - $\text{Al}_2\text{O}_3$ . Feed: 2000 ppmV  $\text{CH}_4$ , 10%  $\text{O}_2$ , 50 ppmV  $\text{SO}_2$ , balance  $\text{N}_2$ .



**Qinghu Tang, Yuanting Chen, Yanhui Yang***Journal of Molecular Catalysis A: Chemical* 315 (2010) 43

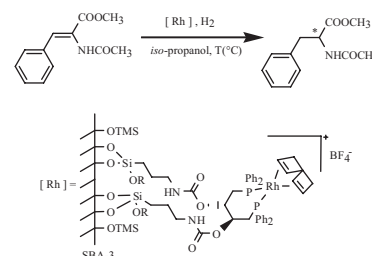
Understanding the nature of vanadium species supported on activated carbon and its catalytic properties in the aerobic oxidation of aromatic alcohols

Vanadium oxide catalysts supported on activated carbon (V/AC) were prepared. The catalytic activity for the benzyl alcohol aerobic oxidation largely depended on the dispersion, oxidation state, and local coordination of vanadium oxides on activated carbon support. Highly dispersed vanadium (5+) species with a distorted tetrahedral coordination were postulated to account for the excellent catalytic performances of V/AC catalysts.

**Reine Sayah, Marie Le Floch, Eric Framery, Véronique Dufaud***Journal of Molecular Catalysis A: Chemical* 315 (2010) 51

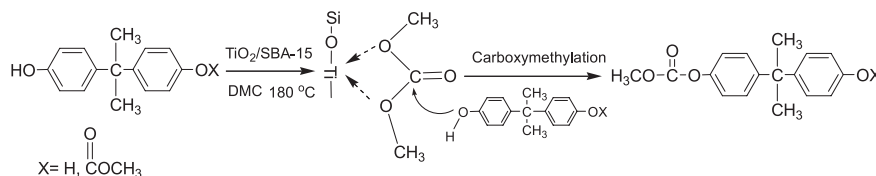
Immobilization of chiral cationic diphosphine rhodium complexes in nanopores of mesoporous silica and application in asymmetric hydrogenation

Heterogeneous chiral cationic rhodium complexes bearing bidentate phosphine derived from (-)-2,2-dimethyl-4,5-bis(diphenylphosphino)methyl-1,3-dioxolane (DIOP) were prepared by covalent immobilization onto SBA type silica. Their performances were then evaluated in the hydrogenation of methyl (Z)-2-N-acetylaminocinnamate.

**Kunmei Su, Zhenhuan Li, Bowen Cheng, Kun liao, Dexin Shen, Yufei Wang***Journal of Molecular Catalysis A: Chemical* 315 (2010) 60

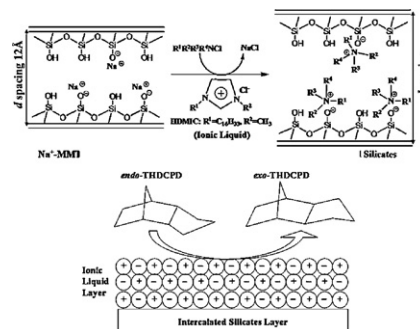
Studies on the carboxymethylation and methylation of bisphenol A with dimethyl carbonate over TiO<sub>2</sub>/SBA-15

Carboxymethylated species were synthesized from dimethyl carbonate (DMC) and bisphenol A (BPA) over TiO<sub>2</sub>/SBA-15, and Si-O-Ti was active sites for reaction. When DMC was attacked by Ti-O-Si on CH<sub>3</sub>-O moiety, BPA attacked carbonyl carbon to form carboxymethylated products. Chemisorbed H<sub>2</sub>O over TiO<sub>2</sub>/SBA-15 made DMC to act as methylating agent. After chemisorbed H<sub>2</sub>O was removed, carboxymethylated species were selectively synthesized.

**Ming-Yu Huang, Jung-Chung Wu, Fuh-Sheng Shieu, Jiang-Jen Lin***Journal of Molecular Catalysis A: Chemical* 315 (2010) 69

Isomerization of *endo*-tetrahydrodicyclopentadiene over clay-supported chloroaluminate ionic liquid catalysts

The intercalation of quaternary halide ionic liquids (ILs) to the layered MMT clay enlarged the silicate spacing and altered the clay hydrophilic to hydrophobic property. The IL-intercalated MMT was subsequently used to support the chloroaluminate ionic liquid for catalyzing the cycloalkane isomerization.

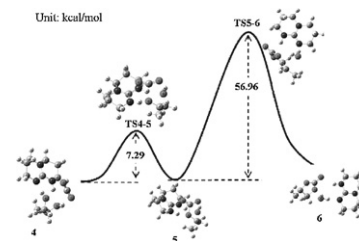


**Jun Ma, Xuelan Zhang, Ning Zhao, Abdullah S.N. Al-Arifi, Taieb Aouak, Zeid Abdullah Al-Othman, Fukui Xiao, Wei Wei, Yuhuan Sun**

*Journal of Molecular Catalysis A: Chemical* 315 (2010) 76

Theoretical study of TBD-catalyzed carboxylation of propylene glycol with CO<sub>2</sub>

Density functional theory method was employed to study the reaction of propylene glycol (PG) and CO<sub>2</sub> with 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD) as the catalyst. Calculations indicate that PG-activated route was the most probable reaction path, and the rate-determining step was the nucleophilic attack of O in CO<sub>2</sub> on the C in PG with energy barrier 56.96 kcal/mol.

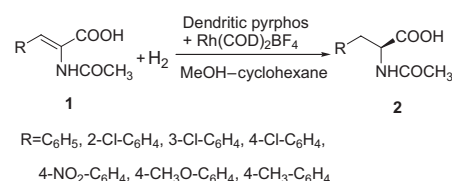


**Bing Yi, Hua-Ping He, Qing-Hua Fan**

*Journal of Molecular Catalysis A: Chemical* 315 (2010) 82

Synthesis and application of peripherally alkyl-functionalized dendritic pyrphos ligands: Homogeneous-supported catalysts for enantioselective hydrogenation

Peripherally alkyl-functionalized dendritic pyrphos ligands have been synthesized and employed in the Rh-catalyzed asymmetric hydrogenation. The second-generation dendritic catalyst could be recycled via a liquid-liquid biphasic separation method.

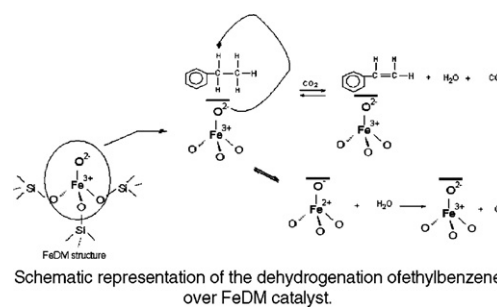


**Andressa H. de Morais Batista, Francisco F. de Sousa, Sara B. Honorato, Alejandro P. Ayala, Josue M. Filho, Francisco W. de Sousa, Antonio N. Pinheiro, J.C.S. de Araujo, Ronaldo F. Nascimento, Antoninho Valentini, Alcineia C. Oliveira**

*Journal of Molecular Catalysis A: Chemical* 315 (2010) 86

Ethylbenzene to chemicals: Catalytic conversion of ethylbenzene into styrene over metal-containing MCM-41

The Fe<sup>3+</sup> acid site of the catalyst adsorbs ethylbenzene, reversibly abstracting the α-hydrogen at a basic OH adjacent to the acid site. The base sites, e.g., oxygen species and O<sup>-</sup> species, activate the gaseous CO<sub>2</sub> to form an O<sup>-</sup> entity, which abstracts the β-hydrogen to produce styrene.



**Eunyoung Sin, Song-Se Yi, Yoon-Sik Lee**

*Journal of Molecular Catalysis A: Chemical* 315 (2010) 99

Chitosan-g-mPEG-supported palladium (0) catalyst for Suzuki cross-coupling reaction in water

A chitosan-g-mPEG-supported palladium (0) catalyst has been developed for the Suzuki cross-coupling reaction in neat water. The catalyst showed good catalytic activity with the function of solubilizing the organic substrates by grafted PEG in the reaction. Also, the catalyst was reused up to five times and easily recovered even though its catalytic activity was somehow decreased during the reaction.

