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## Journal of Molecular Catalysis A: Chemical

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## Contents

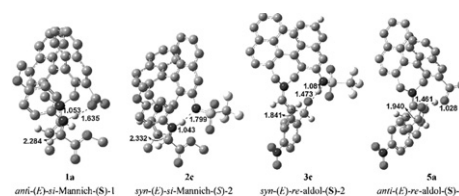
## Articles

**Aiping Fu, Hongliang Li, Tianshu Chu,  
Hanxun Zou, Peng Feng, Shuping Yuan,  
Yunbo Duan**

*Journal of Molecular Catalysis A: Chemical 314 (2009) 1*

Theoretical studies of stereoselectivities in the direct *anti*-Mannich and *syn*-aldol reactions catalyzed by axially chiral amino sulfonamide

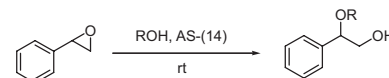
The origins of the stereoselectivities in the axially chiral amino acid (S)-1 and amino sulfonamide (S)-2-catalyzed direct Mannich and aldol reactions have been studied theoretically. The most stable transition states of the crucial C–C bond-forming steps for the Mannich and aldol reactions provide a good explanation for the opposite diastereoselectivities of the above two catalysts.



**Mathew W.C. Robinson, A. Matthew Davies,  
Ian Mabbett, David C. Apperley, Stuart H. Taylor,  
Andrew E. Graham**

*Journal of Molecular Catalysis A: Chemical 314 (2009) 10*

Synthesis and catalytic activity of nanoporous aluminosilicate materials

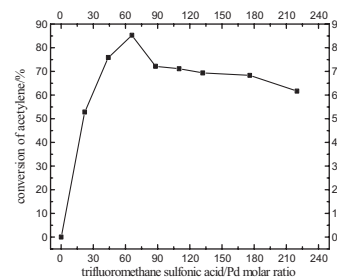


**Cong-Ming Tang, Yi Zeng, Xian-Gui Yang,  
Yong-Cheng Lei, Gong-Ying Wang**

*Journal of Molecular Catalysis A: Chemical 314 (2009) 15*

The palladium catalyzed hydrocarboxylation of acetylene with carbon monoxide to acrylic acid under mild conditions

Carbonylation of acetylene with carbon monoxide to acrylic acid has been investigated using a palladium catalyst system under mild conditions. Among all ligands as used, only diphenyl-2-pyridylphosphine has a good catalytic activity. Sulfonic acids and trifluoroacetic acid as acidic promoters display an excellent performance. Other parameters have also been discussed.

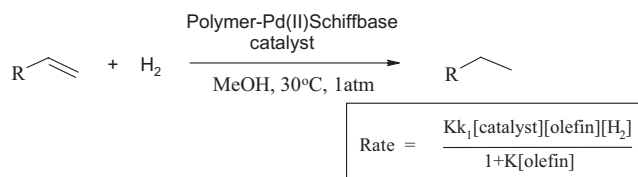


**S. Alexander, V. Udayakumar, V. Gayathri**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 21

Hydrogenation of olefins by polymer-bound palladium(II) Schiff base catalyst

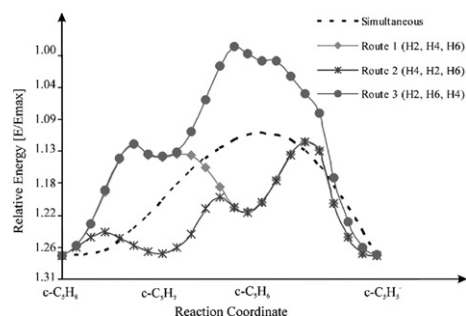
A palladium catalyst was synthesized by modifying chloromethylated poly(styrene-divinylbenzene) into a coordinating Schiff base ligand which was complexed with palladium chloride. The activity of the catalyst was investigated towards hydrogenation of olefins under ambient conditions of temperature and pressure. The polymer-bound catalyst was found to be superior to its homogeneous counter part in its stability and reusability.



**Estefanía Germán, Ignacio López-Corral, Alfredo Juan, Graciela Brizuela**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 28

A theoretical study of cyclopentene ( $c\text{-C}_5\text{H}_8$ ) dehydrogenation to cyclopentadienyl anion ( $c\text{-C}_5\text{H}_5^-$ ) on Ni (1 1 1)

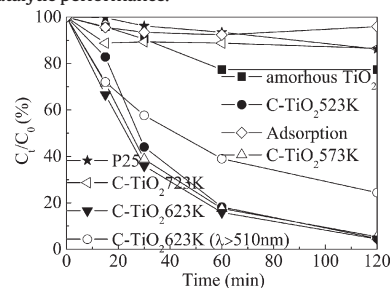


**Chao Chen, Mingce Long, Hui Zeng, Weimin Cai, Baoxue Zhou, Jingyi Zhang, Yahui Wu, Dawei Ding, Deyong Wu**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 35

Preparation, characterization and visible-light activity of carbon modified  $\text{TiO}_2$  with two kinds of carbonaceous species

A novel and simple method was used to synthesize visible-light responsive carbon modified  $\text{TiO}_2$ , which possesses excellent stability and high photocatalytic performance. Carbon elements in the sample calcined at  $350^\circ\text{C}$  simultaneously present as interstitial carbon in the crystal lattice and graphite-like carbon on the surface. And graphite-like carbon contributes greatly to the high photocatalytic performance.

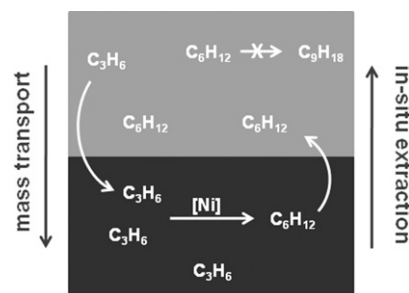


Scheme: Degradation of methyl orange with photocatalyst

**Marcus Eichmann, Wilhelm Keim, Marco Haumann, Berthold U. Melcher, Peter Wasserscheid**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 42

Nickel catalyzed dimerization of propene in chloroaluminate ionic liquids: Detailed kinetic studies in a batch reactor

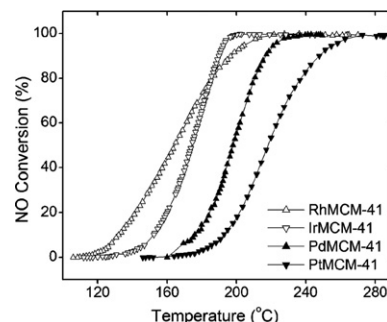


**Vilas Ravat, Dinesh B. Mantri, P. Selvam, Preeti Aghalayam**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 49

Platinum group metals substituted MCM-41 molecular sieves: Synthesis, characterization and application as novel catalysts for the reduction of NO by CO

Mesoporous MCM-41 molecular sieves with Si/M (molar) ratios of 100 containing platinum group metals were synthesized hydrothermally. These catalysts were systematically characterized by various analytical and spectroscopic techniques. The study revealed that catalytic activity for the reduction of NO by CO is in the order Rh > Ir > Pd > Pt, as seen in the figure below.

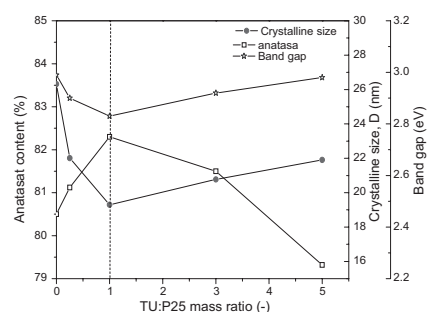


**H. Znad, Y. Kawase**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 55

Synthesis and characterization of S-doped Degussa P25 with application in decolorization of Orange II dye as a model substrate

S-doped P25 photocatalyst with different TU:P25 mass ratios of 0:1, 0.25:1, 1:1, 3:1 and 5:1 have been prepared. The photocatalytic activity of the prepared S-doped P25 was examined by photo-decolorization of azo dye Orange II under natural solar light irradiation. XRD, UV-vis spectroscopy, XPS, SEM and TEM were used to characterize the catalyst. The results showed that the S-doped P25 catalyst at mass ratio of (1:1) and calcinated at 550 °C for 4 h exhibited the highest photocatalytic activity under solar light irradiation. We suggest that Degussa P25 could be used as a Ti precursor for further improving its activity under natural solar light.

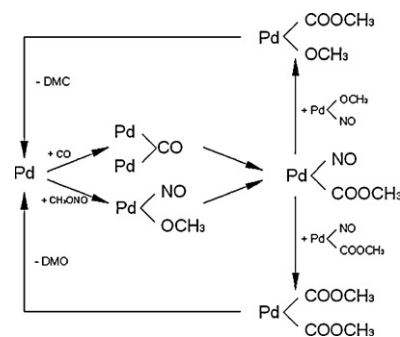


**Yang Ji, Gang Liu, Wei Li, Wende Xiao**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 63

The mechanism of CO coupling reaction to form dimethyl oxalate over Pd/α-Al<sub>2</sub>O<sub>3</sub>

The formation of dimethyl oxalate (DMO) is initiated by adsorptions of methyl nitrite (MN) and CO. Adsorbed species of reactants participated in the reaction are ON-Pd-OCH<sub>3</sub> and bridge bonded CO. The formation of by-product dimethyl carbonate (DMC) is suppressed when the ratio of ON-Pd-OCH<sub>3</sub> to bridge bonded CO over catalysts surface is low.

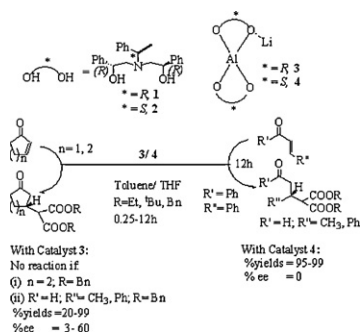


**Neelima D. Tangellamudi, Sundararajan Govindarajan**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 71

Unexpected chemoselectivity of cyclic enones on introducing additional chirality in diethanolamine ligand in catalytic asymmetric Michael addition reactions using heterobimetallics

A homochiral Al-Li heterobimetallic complex of diethanolamine was found to catalyze Michael addition reactions displaying high chemoselectivity with certain Michael acceptors and Michael donors. The heterochiral complex with stereochemical switch on the ligand displayed substrate generality. Herein we give the proposed mechanism and the effect of reversing the order of addition of substrates in causing the reversal of chemoselectivity.

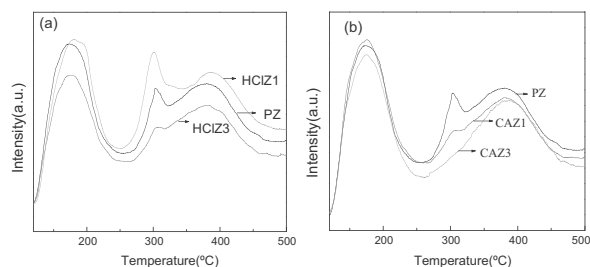


**Xuefeng Bai, Keyi Sun, Wei Wu, Pengfei Yan, Jie Yang**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 81

Methylation of naphthalene to prepare 2,6-dimethylnaphthalene over acid-dealuminated HZSM-12 zeolites

The low concentration of hydrochloric acid removed the aluminum oxide species, which block the micropores, therefore, more acid sites are exposed. The high concentration of hydrochloric acid eliminates the same number of weak and strong acid sites, simultaneously. In contrast, citric acid preferentially eliminates the strong acid sites. By prolonging the dealumination time, the weak acid sites also begin to decrease.

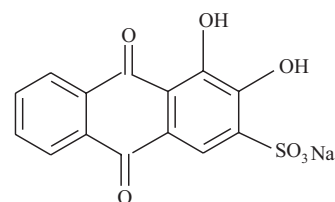


**L. Gomathi Devi, K.E. Rajashekhar, K.S. Anantha Raju, S. Girish Kumar**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 88

Kinetic modeling based on the non-linear regression analysis for the degradation of Alizarin Red S by advanced photo Fenton process using zero valent metallic iron as the catalyst

An approach to kinetic/mathematical model based on the non-linear regression analysis for the degradation of Alizarin Red S by advanced photo Fenton process.

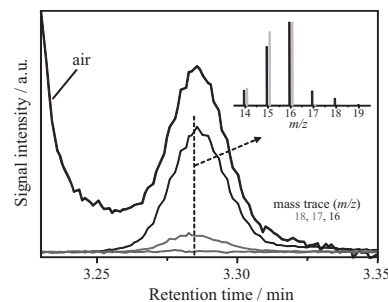


**Seyed Alireza Sadat Rezai, Frank Bauer, Ulrich Decker, Yvonne Traa**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 95

Isotopic studies on the dehydroalkylation of toluene with ethane

The mechanism of dehydroalkylation of toluene with ethane was studied using CD<sub>3</sub>-labeled toluene. Extensive H/D exchange without formation of CD<sub>3</sub>H and interplay of several reactions were observed.



**Hanna Härelind Ingelsten, Anders Hellman, Hannes Kannisto, Henrik Grönbeck**

*Journal of Molecular Catalysis A: Chemical* 314 (2009) 102

Experimental and theoretical characterization of NO<sub>x</sub> species on Ag/α-Al<sub>2</sub>O<sub>3</sub>

The adsorption of NO<sub>x</sub> species on α-alumina and Ag/α-alumina is investigated by *in situ* diffuse reflection infrared Fourier transform (DRIFT) spectroscopy and density functional theory (DFT) calculations.

