



Contents

Articles

G. C. Lloyd-Jones

Journal of Molecular Catalysis A: Chemical 311 (2009) viii

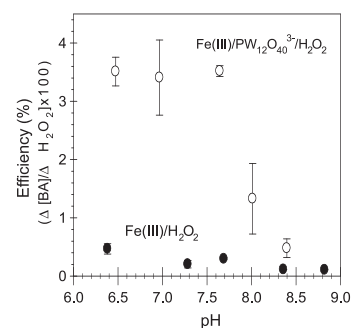
Editorial

Changha Lee, David L. Sedlak

Journal of Molecular Catalysis A: Chemical 311 (2009) 1

A novel homogeneous Fenton-like system with Fe(III)–phosphotungstate for oxidation of organic compounds at neutral pH values

The addition of phosphotungstate ($\text{PW}_{12}\text{O}_{40}^{3-}$) enhances the efficiency of the Fe(III)/ H_2O_2 system at neutral pH values.

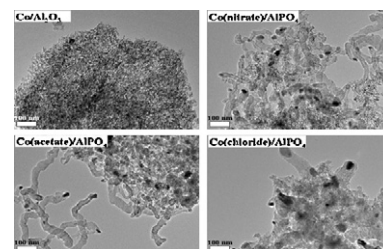


Jong Wook Bae, Seung-Moon Kim, Suk-Hwan Kang, Komandur V.R. Chary, Yun-Jo Lee, Hyo-Jin Kim, Ki-Won Jun

Journal of Molecular Catalysis A: Chemical 311 (2009) 7

Effect of support and cobalt precursors on the activity of Co/AlPO₄ catalysts in Fischer–Tropsch synthesis

Cobalt catalysts supported on amorphous aluminum phosphate (AlPO₄) were prepared by using three different cobalt precursors to elucidate the activity of Fischer–Tropsch synthesis (FTS). The differences in catalytic properties of Co/AlPO₄ are attributed to the cobalt particle size, reducibility and formation of filamentous carbon.

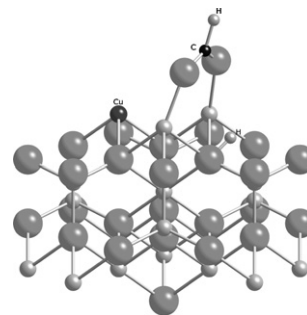


**Rainee M. Van Natter, John S. Coleman,
Carl R.F. Lund**

Journal of Molecular Catalysis A: Chemical 311 (2009) 17

A DFT study of the effect of copper promotion upon iron oxide surface species

A DFT Study of the Effect of Copper Promotion upon Iron Oxide Surface Species, R. M. Van Natter, J. S. Coleman and C. R. F. Lund, Department of Chemical and Biological Engineering, University at Buffalo, SUNY, Buffalo, NY, USA 14260-4200. Adsorption of water-gas shift intermediates on active sites on iron oxide and copper-promoted iron oxide were compared using density functional theory. Relative to the unpromoted catalyst, the strength of adsorption on the promoted catalyst was weakened by less than 20 kJ⁻¹ when copper-substituted below the surface. It was weakened by 60–80 kJ mol⁻¹ when copper-substituted in the surface of the catalyst.

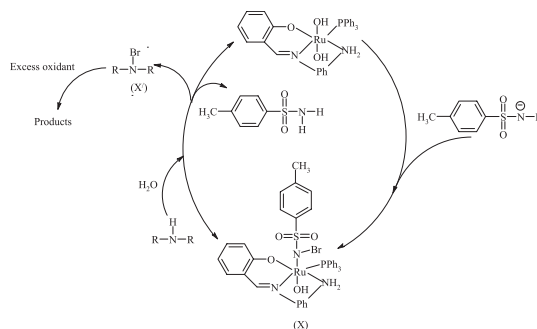


**C.H. Vinod Kumar, K.N. Shivananda,
Rajenahally V Jagadeesh, C. Naga Raju**

Journal of Molecular Catalysis A: Chemical 311 (2009) 23

Ruthenium complex catalyzed oxidative conversion of aliphatic amines to carboxylic acids using bromamine-T: Kinetic and mechanistic study

Ruthenium(III) complex catalyzed oxidation of aliphatic amines with bromamine-T under alkaline condition was performed efficiently to afford carboxylic acids in high conversion. The detailed kinetic and mechanistic investigations have been made. The related rate law has been deduced. Mechanism of amine oxidation is as shown in the following scheme.

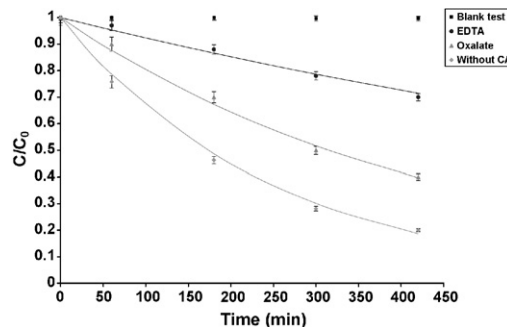


**Xiaofei Xue, Khalil Hanna, Christelle Despas,
Feng Wu, Nansheng Deng**

Journal of Molecular Catalysis A: Chemical 311 (2009) 29

Effect of chelating agent on the oxidation rate of PCP in the magnetite/H₂O₂ system at neutral pH

The H₂O₂ decomposition rate decreased from 0.004 min⁻¹ to 0.0022 min⁻¹ when oxalate is previously sorbed on the magnetite surface and to 0.0008 min⁻¹ when it is EDTA.

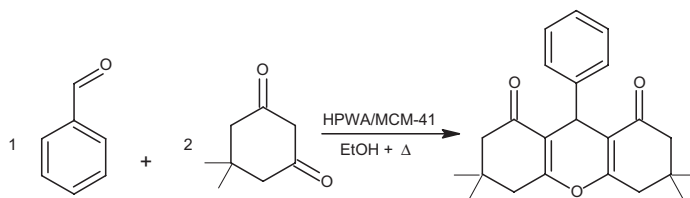


G. Karthikeyan, A. Pandurangan

Journal of Molecular Catalysis A: Chemical 311 (2009) 36

Heteropolyacid (H₃PW₁₂O₄₀) supported MCM-41: An efficient solid acid catalyst for the green synthesis of xanthenedione derivatives

HPWA/MCM-41 mesoporous molecular sieves of appropriate ratios were prepared by the wet impregnation method. The prepared HPWA/MCM-41 materials were characterized by XRD analysis, BET method, FT-IR measurements and TEM technique. The catalytic behaviour of the catalysts was tested for the condensation of dimedone (active methylene carbonyl compound) and various aromatic aldehydes.

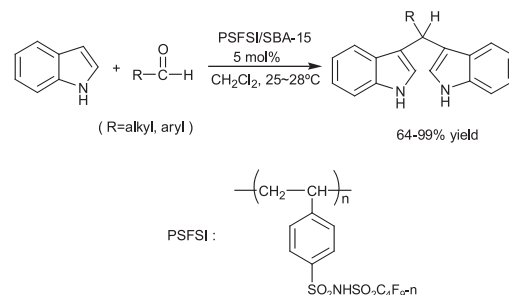


Zhong-Hua Ma, Hong-Bo Han, Zhi-Bin Zhou, Jin Nie

Journal of Molecular Catalysis A: Chemical 311 (2009) 46

SBA-15-supported poly (4-styrenesulfonyl (perfluorobutylsulfonyl) imide) as heterogeneous Brønsted acid catalyst for synthesis of diindolylmethane derivatives

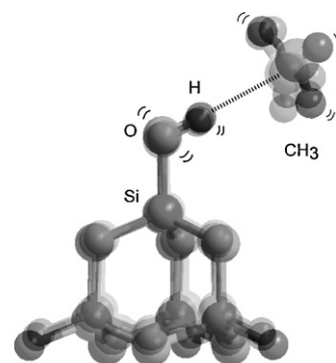
By means of immobilizing the acidic polymer, poly(4-styrenesulfonyl(perfluorobutylsulfonyl)imide) (PSFSI), onto mesoporous SBA-15 silica, a new type of strongly acidic composite catalyst was developed as an effective and reusable solid acid catalyst for the synthesis of diindolylmethane derivatives (DIMs). The properties of the catalyst were characterized by NMR, FT-IR, XRD, SEM, TEM, XPS, TG/DTA, and GPC.



Tomoya Takada, Hiroto Tachikawa

Journal of Molecular Catalysis A: Chemical 311 (2009) 54

DFT and direct ab-initio MD study on hyperfine coupling constants of methyl radicals adsorbed on model surface of silica gel



Olga V. Turova, Eugenia V. Starodubtseva, Maxim G. Vinogradov, Vladimir A. Ferapontov

Journal of Molecular Catalysis A: Chemical 311 (2009) 61

Kinetic study of asymmetric hydrogenation of methyl levulinate using the (COD)Ru(2-methylallyl)₂-BINAP-HCl catalytic system

The kinetics of asymmetric hydrogenation of methyl levulinate in the presence of the (COD)Ru(2-methylallyl)₂-BINAP-HCl catalytic system was studied. The kinetic order in H₂, as well as in the catalyst, was found to be equal to 1, whereas the kinetic order in the substrate and HCl fell from 1 to 0 with increasing their starting concentration. Based on the kinetic and ³¹P NMR data, the most probable mechanism of ruthenium-catalyzed hydrogenation of γ -ketoesters has been suggested.

