

Journal of Molecular Catalysis A: Chemical

journal homepage: www.elsevier.com/locate/molcata

Contents

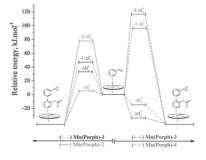
Articles

Rodrigo De Paula, Mário M.Q. Simões, M. Graça P.M.S. Neves, José A.S. Cavaleiro

Journal of Molecular Catalysis A: Chemical 345 (2011) 1

Oxidation of styrene and of some derivatives with H_2O_2 catalyzed by novel imidazolium-containing manganese porphyrins: A mechanistic and thermodynamic interpretation

► Thermodynamic activation parameters are affected by catalysts structural differences. ► Structural differences also change products' selectivity. ► Hammett analysis provided small ρ -values. ► Results fit with a concerted reaction pathway, starting from an oxene-type approach. ► The determining step is a $[\pi 2_a + \pi 2_s]$ metal-looxetane intermediate.



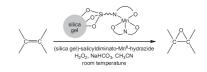
CATAL

Massomeh Ghorbanloo, Hassan Hosseini Monfared, Christoph Janiak

Journal of Molecular Catalysis A: Chemical 345 (2011) 12

The catalytic function of a silica gel-immobilized Mn(II)-hydrazide complex for alkene epoxidation with $\rm H_2O_2$

► A Mn(II)-hydrazone complex has been anchored on the surface of a silica gel. ► This com-pound is a stable and recyclable heterogeneous catalyst. ► This catalyst is a very active in epox-idation reactions with $H_2O_2/CH_3CN/NaHCO_3$. ► Cycloalkenes were oxidized to their epoxides with excellent selectivity. ► This catalytic system showed good activities in the epoxidation of linear alkenes.

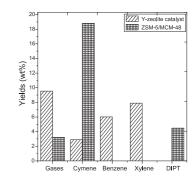


T. Odedairo, R.J. Balasamy, S. Al-Khattaf

► Mesopores containing ZSM-5 is reported for alkylation and cracking reactions. ► Presence of mesopores led to a high 1,3,5-TIPB conversion. ► Acidity as well as pore size of catalysts plays a crucial role in the cracking reaction.

Journal of Molecular Catalysis A: Chemical 345 (2011) 21

Influence of mesoporous materials containing ZSM-5 on alkylation and cracking reactions

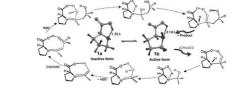


Manjaly J. Ajitha, Cherumuttathu H. Suresh

Journal of Molecular Catalysis A: Chemical 345 (2011) 37

A higher energy conformer of (S)-proline is the active catalyst in intermolecular aldol reaction: Evidence from DFT calculations

► Theoretical revisiting of (*S*)-proline catalyzed intermolecular aldol reaction. ► Higher energy conformer of (*S*)-proline is found to be the active catalyst. ► The mechanism passes through eight proton transfer transition states. ► Hydrogen bond catalysis.

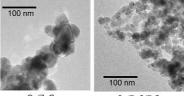


Yasuyuki Matsumura, Hideomi Ishibe

Journal of Molecular Catalysis A: Chemical 345 (2011) 44

Effect of zirconium oxide added to Cu/ZnO catalyst for steam reforming of methanol to hydrogen

► Addition of ZrO₂ to Cu/ZnO improves the activity to methanol steam reforming. ► Addition of ZrO₂ reduces particle sizes of Cu and ZnO. ► ZrO₂ does not directly enhance surface activity of Cu/ZnO/ZrO₂. ► Strong contact between Cu and ZnO particles increases activity. ► ZrO₂ particles mitigate structural change of Cu and ZnO at 400°C.



Cu/ZnO

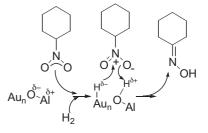
Cu/ZnO/ZrO

Ken-ichi Shimizu, Takumi Yamamoto, Yutaka Tai, Atsushi Satsuma

Journal of Molecular Catalysis A: Chemical 345 (2011) 54

Selective hydrogenation of nitrocyclohexane to cyclohexanone oxime by alumina-supported gold cluster catalysts

► Au/Al₂O₃ shows higher selectivity of cyclo-hexanone oxime than the standard Au catalyst, Au/TiO₂. ▶ This is the first successful example of heterogeneous Au catalyst for the title reaction. ▶ Smaller Au size and acid–base bifunctional support result in higher catalytic efficiency. ► Mechanistic studies suggest a cooperation of AuCUS sites and the acid-base pair site of Al₂O₂.

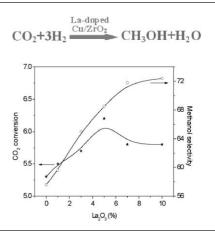


Xiaoming Guo, Dongsen Mao, Guanzhong Lu, Song Wang, Guisheng Wu

Journal of Molecular Catalysis A: Chemical 345 (2011) 60

The influence of La doping on the catalytic behavior of Cu/ZrO₂ for methanol synthesis from CO₂ hydrogenation

► The presence of La favors the production of methanol. The introduction of La affects the Cu surface area of catalyst. ► The introduction of La affects the basicity of catalyst. \blacktriangleright A linear relationship exists between CO₂ conversion and the Cu surface area. ► The methanol selectivity is related to the distribution of basic sites of catalyst.



Vinícius V. Costa, Kelly A. da Silva Rocha, Líniker F. de Sousa, Patricia A. Robles-Dutenhefner, Elena V. Gusevskaya

Journal of Molecular Catalysis A: Chemical 345 (2011) 69

Isomerization of α -pinene oxide over cerium and tin catalysts: Selective synthesis of trans-carveol and trans-sobrerol

Ferenc Lónyi, Hanna E. Solt, József Valyon,

Journal of Molecular Catalysis A: Chemical 345 (2011) 75

The activation of NO and CH₄ for NO-SCR reaction over In- and Co-containing H-ZSM-5 catalysts

Alicia Boix, Laura B. Gutierrez

▶ Mesoporous molecular sieves Sn/SiO₂ and Ce/SiO₂ were prepared by a sol-gel method. ▶ Both materials catalyze the liquid-phase isomerization/hydration of α -pinene oxide. \blacktriangleright Reaction selectivity is determined by the polarity and basicity of the solvent. ► In weakly basic acetone, the reactions gave *trans*-sobrerol in high yields. ► In dimethylacetamide, which is a basic solvent, the main product was *trans*-carveol.

► InO⁺/In⁺ redox couple is the NO-SCR active site of In,H-zeolites. ► Methane is activated for NO-SCR over zeolite-bound NO⁺ and NO₂[−] surface intermediates. ► Surface intermediates are formed in reaction of NO/NO₂ and In,H-zeolite. > Zeolite Brønsted acid sites promote NO/NO₂ formation from NO/O₂ (NO-COX reaction) ► Co-oxide additive enhances the NO-COX activity of H- and In, H-zeolite catalysts.

Bo Li, Xiaohong Li, Hongna Wang, Peng Wu

Journal of Molecular Catalysis A: Chemical 345 (2011) 81

Pt nanoparticles entrapped in ordered mesoporous carbon for enantioselective hydrogenation

► CMK-3 ordered mesoporous carbon as support for Pt nanoparticles. ► Catalysts are effective for heterogeneous asymmetric hydrogenation of α - ketoesters. \blacktriangleright Catalysts are more efficient than the commercial Pt/C catalyst. Catalysts show supe-rior stability to the commercial Pt/Al₂O₃ catalyst.

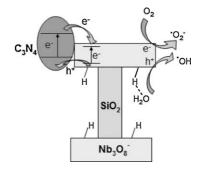
Huiqi Pan, Xiukai Li, Zongjin Zhuang, Chi Zhang

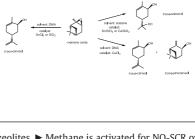
Journal of Molecular Catalysis A: Chemical 345 (2011) 90

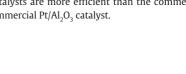
g-C₃N₄/SiO₂-HNb₃O₈ composites with enhanced photocatalytic activities for rhodamine B degradation under visible light

► g-C₃N₄/SiO₂-HNb₃O₈ composites were prepared by solid state reaction. ► g-C₃N₄/SiO₂-HNb₃O₈ composites are visible light active photocatalysts. \triangleright g-C₃N₄/SiO₂-HNb₃O₈ exhibited superior activity than SiO₂-HNb₃O₈ and $g-C_3N_4$. The enhanced activity is ascribed to the synergism between the two components.

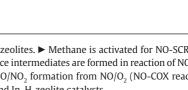
00 h-1 82 29







: BT: 5 m



B.L.A. Prabhavathi Devi, K.N. Gangadhar, K.L.N. Siva Kumar, K. Shiva Shanker, R.B.N. Prasad, P.S. Sai Prasad

Feng Wang, Kan Zhang

rhodamine B

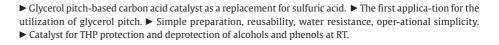
Journal of Molecular Catalysis A: Chemical 345 (2011) 96

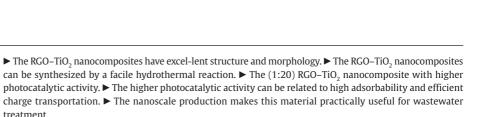
Synthesis of sulfonic acid functionalized carbon catalyst from glycerol pitch and its application for tetrahydropyranyl protection/deprotection of alcohols and phenols

Journal of Molecular Catalysis A: Chemical 345 (2011) 101

Reduced graphene oxide-TiO₂ nanocomposite with

high photocatalystic activity for the degradation of





ROF

= alky, aryl

Dapeng Li, Yilin Tong, Jun Huang, Liyun Ding,

Journal of Molecular Catalysis A: Chemical 345 (2011) 108 First observation of tetranitro iron (II) phthalocyanine catalyzed oxidation of phenolic pollutant assisted with 4-aminoantipyrine using

Yunming Zhong, Dan Zeng, Ping Yan

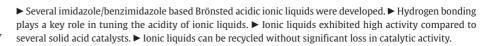
dioxygen as oxidant

► TNFe(II)PC could catalyze oxidation of phenol and chlorophenol pollutant. ► Dioxygen is oxidant and sufficient for the catalytic oxidation reaction. ► Superoxide anion radical is the active species generated in catalytic process. ► Successive single electron transfer is the key step of catalytic mechanism.

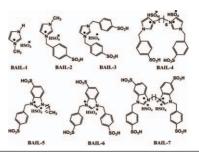
Rajkumar Kore, Rajendra Srivastava

Journal of Molecular Catalysis A: Chemical 345 (2011) 117

Synthesis and applications of novel imidazole and benzimidazole based sulfonic acid group functionalized Brönsted acidic ionic liquid catalysts



catalys





Releved Graphene Oxide-TiO

MeOH