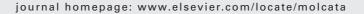


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Journal of Molecular Catalysis A: Chemical





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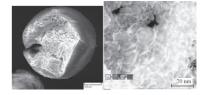
Articles

Samuel P.D. Marques, Anderson L. Pinheiro, Tiago P. Braga, Antoninho Valentini, Josue M. Filho, Alcineia C. Oliveira

Journal of Molecular Catalysis A: Chemical 348 (2011) 1

Nanocasted oxides for oxidative dehydrogenation of ethylbenzene utilizing CO₂ as soft oxidant

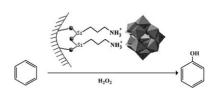
- ► Nanocasted CoFe₂O₄Co₂O₃ and CeO₂ oxides. ► Solids highly actives for styrene production.
- ► Replication of the mold and spherical morphology.



Ali Nemati Kharat, Sayedreza Moosavikia, Bahareh Tamaddoni Jahromi, Alireza Badiei

Journal of Molecular Catalysis A: Chemical 348 (2011) 14

Liquid phase hydroxylation of benzene to phenol over vanadium substituted Keggin anion supported on amine functionalized SBA-15 ▶ In this report we synthesized Keggin type vanadium substituted molybdophosphoric acid supported on amine functionalized SBA-15. ▶ We investigated this catalyst on direct hydroxylation of benzene to phenol in liquid phase. ▶ Under optimized conditions 20% conversion of benzene and 95% selectivity to phenol was achieved.



Nader Ghaffari Khaligh, Farhad Shirini

Journal of Molecular Catalysis A: Chemical 348 (2011) 20

Preparation, characterization and use of poly(4-vinylpyridinium) hydrogen sulfate salt as an ecobenign, efficient and reusable solid acid catalyst for the chemoselective 1,1-diacetate protection and deprotection of aldehydes

- ▶ Introducing the new catalyst (as solid acid) for organic transformations. ▶ Introducing an efficient new method for protection of aldehydes. ▶ Generality of the method, high yields and very short reaction times.
- ► Application of solventfree conditions in the reaction.



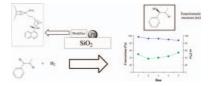
vi Contents

Cristian H. Campos, Marcelo Oportus, Cecilia Torres, Claudia Urbina, José L.G. Fierro, Patricio Reyes

Journal of Molecular Catalysis A: Chemical 348 (2011) 30

Enantioselective hydrogenation of 1-phenyl-propane-1,2-dione on immobilised cinchonidine Pt/SiO₂ catalysts

▶ SiO_2 supports were synthesized by immobilised modified cinchonidine. ▶ Catalysts were prepared at 1% mass Pt supported on modified SiO_2 . ▶ The catalysts are active in enantioselective hydrogenation of 1-phenyl-propane-1,2- dione. ▶ The most enantioselective catalyst is used in recycling test. ▶ All the recycling test show loss of enantioselectivity and activity.



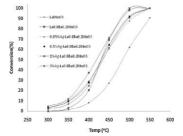
Suresh Kumar, Y. Teraoka, Amish G. Joshi, S. Rayalu, Nitin Labhsetwar

Journal of Molecular Catalysis A: Chemical 348 (2011) 42

Ag promoted $La_{0.8}Ba_{0.2}MnO_3$ type perovskite catalyst for N_2O decomposition in the presence of O_2 , NO and H_2O

► Catalytic activity of LaMnO₃ has been improved by Ba and Ag promotion. ► Ag addition alters the redox properties of perovskite, which is responsible for improved catalytic activity. ► Altered valance states of Mn has been confirmed by XPS studies and corroborated by TPD as well as TPR analysis. ► 1 wt% Ag promoted

 $\label{eq:La08} \begin{array}{l} La_{0.8}Ba_{0.2}MnO_3 \mbox{ shows } 100\% \ N_2O \mbox{ conversion} \\ \mbox{at } 550 \ ^{\rm o}c \mbox{ with a reaction rate of } 0.028 \\ \mbox{mmol } \mbox{g}^{-1} \mbox{ min}^{-1}. \end{array}$

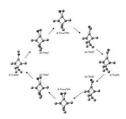


Rodolfo Izquierdo, Leonardo J. Rodríguez, Rafael Añez, Aníbal Sierraalta

Journal of Molecular Catalysis A: Chemical 348 (2011) 55

Direct catalytic decomposition of NO with Cu–ZSM-5: A DFT–ONIOM study

► The use of ONIOM methodologies makes possible a combined quantum mechanism/molecular mechanism calculations in system with hundreds of atoms. ► The DFT calculations provide new insights in the direct DeNO $_{x}$ mechanisms by Cu–ZSM5 systems. ► The species [Cu– κ^{2} NO]* account for the liking species between the twopath mechanism.

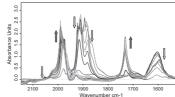


Samuel Jali, Holger B. Friedrich, Gerrit R. Julius

Journal of Molecular Catalysis A: Chemical 348 (2011) 63

The effect of $\mathrm{Mo(CO)_6}$ as a co-catalyst in the carbonylation of methanol to methyl formate catalyzed by potassium methoxide under CO, syngas and $\mathrm{H_2}$ atmospheres. HP-IR observation of the methoxycarbonyl intermediate of $\mathrm{Mo(CO)_6}$

- $\blacktriangleright \text{ The Mo(CO)}_6 \text{ catalyzed production of methyl formate from CH}_3 \text{OH, syngas, CO, H}_2 \text{ and KOCH}_3 \text{ was studied.}$
- ▶ HP-IR studies under CO, syngas, H₂ and N₂ showed that the mechanism goes via [Mo(CO)₅(COOCH₂)]⁻.
- ► $[Mo(CO)_5(COOCH_3)]^-$ is then protonated by methanol to eliminate methyl formate. ► HP-IR results under H_2 and N_2 showed formation of μ -HMo $_2(CO)_{10}^-$ as $[Mo(CO)_5(COOCH_3)]^-$ diminishes. ► The role of methanol in the protonation of the methoxycarbonyl adduct is significant.

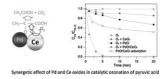


Weiwei Li, Zhimin Qiang, Tao Zhang, Xiaolei Bao, Xu Zhao

Journal of Molecular Catalysis A: Chemical 348 (2011) 70

Efficient degradation of pyruvic acid in water by catalytic ozonation with PdO/CeO₂

► PdO/CeO₂ is an effective catalyst for ozonation of pyruvic acid in water. ► Surface Ce³*/Pd²* molar ratio and metal charging states dominate catalyst activity. ► PdO/CeO₂ catalysis is ascribed to the synergetic effect of Pd and Ce

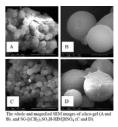


Jinmei Miao, Hui Wan, Yanbing Shao, Guofeng Guan, Bin Xu

Journal of Molecular Catalysis A: Chemical 348 (2011) 77

Acetalization of carbonyl compounds catalyzed by acidic ionic liquid immobilized on silica gel

► Immobilized [(CH₂)₃SO₃H-HIM]HSO₄ prepared by using TEOS as silica source was prepared. ► SG-[(CH₂)₃SO₃H-HIM]HSO₄ exhibited high catalytic activity for acetalization. ► SG-[(CH₂)₃SO₃H-HIM]HSO₄ could be recycled easily and exhibited excellent reusability.

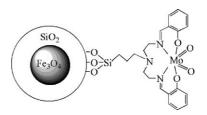


M. Masteri-Farahani, N. Tayyebi

Journal of Molecular Catalysis A: Chemical 348 (2011) 83

A new magnetically recoverable nanocatalyst for epoxidation of olefins

► Silica coated magnetite nanoparticles were modified with a Schiff base ligand. ► Next reaction with MoO₂(acac)₂ afforded MoO₂salpr/SCMNPs. ► The prepared MoO₂salpr/SCMNPs was active in the epoxidation of olefins

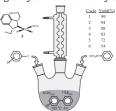


Hayati Türkmen, Levent Pelit, Bekir Çetinkaya

Journal of Molecular Catalysis A: Chemical 348 (2011) 88

 $Water-soluble \it cis-[(NHC)PdBr_2(TPPTS)] catalysts and their applications in Suzuki-Miyaura coupling of arylchlorides$

▶ Water soluble complexes were prepared. ▶ These complexes were active in the Suzuki cross-coupling reactions. ▶ Makes the catalyst reusable. ▶ This process is ecologically and economically acceptable.



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Habib Firouzabadi, Nasser Iranpoor, Faezeh Kazemi

Journal of Molecular Catalysis A: Chemical 348 (2011) 94

Carbon–carbon bond formation *via* homocoupling reaction of substrates with a broad diversity in water using Pd(OAc)₂ and agarose hydrogel as a bioorganic ligand, support and reductant

- ▶ Agarose was used as a reductant for Pd(II) salt. ▶ Agarose was used as a support for palladium particles.
- ▶ Homocoupling reaction of aryl halides was reported. ▶ The reaction was conducted in aqueous media.
- ▶ The reaction was conducted under ligand- and amine-free conditions.

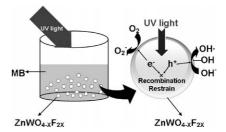
$$R \longrightarrow X \qquad \begin{array}{c} Pd(OAc)_2 \ (0.02 \ mmol) \\ Agarose(0.05 \ g) \\ \hline NaOH \ (1.5 \ mmol) \\ H_2O \ (2 \ mL), \ 90 \ ^{\circ}C \end{array} \qquad R \longrightarrow \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}$$

Guangli Huang, Rui Shi, Yongfa Zhu

Journal of Molecular Catalysis A: Chemical 348 (2011) 100

Photocatalytic activity and photoelectric performance enhancement for ZnWO₄ by fluorine substitution

▶ The formation of fluorine substitution can be attained by a two step process. ▶ Comparing with $ZnWO_4$ the activity of $ZnWO_{4-x}F_{2x}$ almost doubled. ▶ Enhanced activity was attributed to higher density hydroxyl of $ZnWO_{4-x}F_{2x}$ ▶ $ZnWO_{4-x}F_{2x}$ possessed higher donor density and efficiency of charge separation.

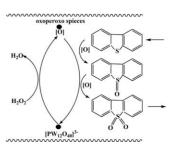


Baoshan Li, Zhenxing Liu, Chunying Han, Jianjun Liu, Shengli Zuo, Zhiyuan Zhou, Xinmei Pang

Journal of Molecular Catalysis A: Chemical 348 (2011) 106

Preparation, characterization and catalytic performance of the silica pillared clay incorporated with phosphotungstic acid using different surfactants as template

▶ HPW heteropoly acid was encapsulated into the mesoporous sillica pillared clay. ▶ Surfactant have a significant impact in the formation of the gallery pore. ▶ The catalysts exhibit high catalytic activity in deep ODS of model oil. ▶ The catalysts exhibit good reusability.



Bin Zhao, Feng Chen, Yanchao Jiao, Hongyun Yang, Jinlong Zhang

Journal of Molecular Catalysis A: Chemical 348 (2011) 114

Ag⁰-loaded brookite/anatase composite with enhanced photocatalytic performance towards the degradation of methyl orange

▶ Ag°-loaded brookite/anatase ${\rm TiO}_2$ with uniform Ag° size distribution was prepared. ▶ 2.0% Ag°-loaded brookite/anatase ${\rm TiO}_2$ has the highest photocatalytic reactivity. ▶ Hetero-junction in brookite/anatase composite benefits the charge separation. ▶ Schottky barrier between Ag° and ${\rm TiO}_2$ further improved the charge separation.

