ELSEVIER

Contents lists available at ScienceDirect

Journal of Molecular Catalysis A: Chemical

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



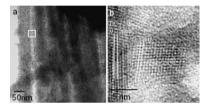
Contents

Articles

Lifeng Cui, Feng Huang, Mutong Niu, Lingwei Zeng, Ju Xu, Yuansheng Wang Nano-composite with Fe-doped anatase TiO₂ nanoparticles coupling with TiO₂(B) nanobelts was prepared by a simple two-step solution synthesis procedure, which exhibits desirable visible light photocatalytic activity.

Journal of Molecular Catalysis A: Chemical 326 (2010) 1

A visible light active photocatalyst: Nano-composite with Fe-doped anatase TiO₂ nanoparticles coupling with TiO₃(B) nanobelts

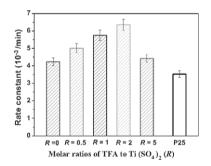


Jiaguo Yu, Lei Shi

Journal of Molecular Catalysis A: Chemical 326 (2010) 8

One-pot hydrothermal synthesis and enhanced photocatalytic activity of trifluoroacetic acid modified ${\rm TiO_2}$ hollow microspheres

Trifluoroacetic acid (TFA) modified TiO_2 hollow microspheres, prepared by one-pot hydrothermal method using $\text{Ti}(\text{SO}_4)_2$ and TFA as precursors, show higher photocatalytic activity than P25 and pure TiO₂.

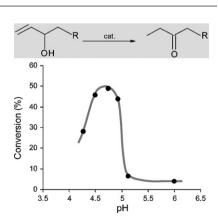


Beatríz González, Pablo Lorenzo-Luis, Manuel Serrano-Ruiz, Éva Papp, Marianna Fekete, Klára Csépke, Katalin Ösz, Ágnes Kathó, Ferenc Joó, Antonio Romerosa

Journal of Molecular Catalysis A: Chemical 326 (2010) 15

Catalysis of redox isomerization of allylic alcohols by $[RuClCp(mPTA)_2](OSO_2CF_3)_2$ and $[RuCp(mPTA)_2(OH_2-\kappa O)](OSO_2CF_3)_3$ ·(H $_2$ O)(C $_4$ H $_10$ O) $_0$ 5. Unusual influence of the pH and interaction of phosphate with catalyst on the reaction rate

The title complexes catalyzed effectively the redox isomerization of alk-1-en-3-ols. A reaction rate maximum against pH, and strong interaction of [RuCl(Cp) (mPTA) $_2$](OSO $_2$ CF $_3$) $_2$ (mPTA: N-methyl-PTA) with phosphate buffer was observed.



vi Contents

Biswajit Deb, Dipak Kumar Dutta

Journal of Molecular Catalysis A: Chemical 326 (2010) 21

Influence of phosphorus and oxygen donor diphosphine ligands on the reactivity of rhodium(I) carbonyl complexes

Four newly synthesized rhodium(I) carbonyl complexes of phosphorus and oxygen donor diphosphine ligands exhibit higher catalytic activity (TON 679–1768) than Monsanto's species (TON 463–1000) under similar experimental conditions.

$$CH_{3}OH + CO$$

$$CH_{2}OH + CO$$

$$Cat: (Rh(CO)C(L)), (Rh(CO)_{2}C(L^{2}))$$

$$L \approx \sum_{Ph^{-P}, Ph, Ph^{-P}, Ph} L^{P} = \sum_{Ph^{-P}, Ph, Ph} L^{P} + \sum_{Ph^{-P}, Ph} L^{P} = \sum_{Ph^{-P}, Ph} L^{P}$$

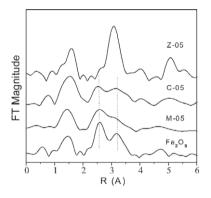
$$X = None \text{ or } C(CH_{3})_{2}$$

Hulin Wang, Yong Yang, Jian Xu, Hong Wang, Mingyue Ding, Yongwang Li

Journal of Molecular Catalysis A: Chemical 326 (2010) 29

Study of bimetallic interactions and promoter effects of FeZn, FeMn and FeCr Fischer-Tropsch synthesis catalysts

EXAFS results show Mn and Cr atoms are incorporated into the lattice of $\alpha\text{-Fe}_2\text{O}_3$, while for Zn promoter, the phase separation and reconstruction are observed and ZnFe $_2\text{O}_4$ compound appeares.



Donghui Wei, Wenjing Zhang, Yanyan Zhu, Mingsheng Tang

Journal of Molecular Catalysis A: Chemical 326 (2010) 41

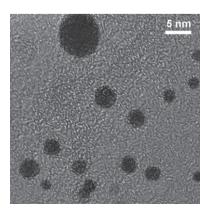
A DFT study on the reaction mechanisms of keteneketone [2 + 2 + 2] cycloaddition to form 3aryglutaric anhydrides under a Lewis acid catalysis: What is the role of BF₃? Why can **R1** react with **R2** to generate **P** under the BF_3 -catalyzed condition? What is the role of Lewis acid BF_3 ? In this paper, we have investigated the mechanisms of the title reaction.

Fernando Cárdenas-Lizana, Zahara M. de Pedro, Santiago Gómez-Quero, Mark A. Keane

Journal of Molecular Catalysis A: Chemical 326 (2010) 48

Gas phase hydrogenation of nitroarenes: A comparison of the catalytic action of titania supported gold and silver

Au/TiO₂ and Ag/TiO₂ (see TEM image) are 100% selective in the hydrogenation of *para*-substituted nitroarenes to the corresponding amine: Hammet treatment of reaction kinetics is consistent with a nucleophilic mechanism.



Contents vii

Hossein A. Dabbagh, Keivan Taban, Mehdi Zamani

Journal of Molecular Catalysis A: Chemical 326 (2010) 55

Effects of vacuum and calcination temperature on the structure, texture, reactivity, and selectivity of alumina: Experimental and DFT studies The effect of vacuum on the structure and texture of alumina was examined. Dehydration mechanism of (R)-, (S)-2-octanol and (R)-, (S)-DPP over $(1\ 0\ 0)$ surface alumina was computed using DFT.



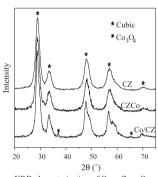


Guangfeng Li, Qiuyan Wang, Bo Zhao, Renxian Zhou

Journal of Molecular Catalysis A: Chemical 326 (2010) 69

Modification of Ce_{0.67}Zr_{0.33}O₂ mixed oxides by coprecipitated/impregnated Co: Effect on the surface and catalytic behavior of Pd only three-way catalyst

Figure displays the XRD patterns of samples. It is noting that the introduction of Co by co-precipitation enters into the ceria–zirconia lattice and forms the homogeneous ternary solid solution.



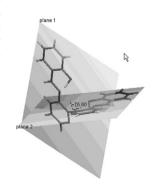
XRD characterization of Ce_{0.67}Zr_{0.33}O₂ mixed oxides doped by cobalt oxide.

Murat Aydemir, Feyyaz Durap, Akın Baysal, Nermin Meric, Ayşegül Buldağ, Bahattin Gümgüm, Saim Özkar, Leyla Tatar Yıldırım

Journal of Molecular Catalysis A: Chemical 326 (2010) 75

Novel neutral phosphinite bridged dinuclear ruthenium(II) arene complexes and their catalytic use in transfer hydrogenation of aromatic ketones: X-ray structure of a new Schiff base, N3,N3'-di-2-hydroxybenzylidene-[2,2']bipyridinyl-3,3'-diamine

A novel Schiff base N3,N3'-di-2-hydroxybenzylidene-[2,2']bipyridinyl-3,3'-diamine and its bis(phosphinite) dinuclear ruthenium(II) complexes $[C_{24}H_{16}N_4\{OPPh_2-Ru(\eta^6-benzene)Cl_2\}_2]$ and $[C_{24}H_{16}N_4\{OPPh_2-Ru(\eta^6-pcymene)Cl_2\}_2]$ were prepared and characterized. These complexes were evaluated in the ruthenium-catalyzed transfer hydrogenation of ketones.



Zongwen Guo, Weitao Huo, Mingjun Jia, Kaige Li, Zhenlu Wang, Wenxiang Zhang

Journal of Molecular Catalysis A: Chemical 326 (2010) 82

Hydrodealkylation of 1,2,4-trimethylbenzene over reduced Ni–Al mixed oxide catalysts prepared by co-precipitation method Partially reduced Ni–Al mixed oxide catalysts exhibit high activity for the hydrodealkylation of 1,2,4-TMB. The neighboring metallic Ni(0) atoms and the Lewis acidic sites may play a synergic role.

$$+ H_2 \xrightarrow{\text{Ni-Al Pseudo-spinel}} + CH_4$$

viii Contents

Delian Yi, Hailu Zhang, Zongwu Deng

Journal of Molecular Catalysis A: Chemical 326 (2010) 88

¹H and ¹⁵N chemical shifts of adsorbed acetonitrile as measures to probe the Brønsted acid strength of solid acids: A DFT study

Correlations between $^{1}\mathrm{H}$ or $^{15}\mathrm{N}$ chemical shift of acetonitrile/Brønsted acid adsorption complexes and acid strength of Brønsted acid site have been derived by DFT calculation.

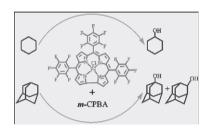


Achintesh Narayan Biswas, Purak Das, Arunava Agarwala, Debkumar Bandyopadhyay, Pinaki Bandyopadhyay

Journal of Molecular Catalysis A: Chemical 326 (2010) 94

Selective hydroxylation of alkanes catalyzed by iron(IV)corrole

The complex meso-tris(pentafluorophenyl)corrolatoiron (IV)chloride [(F_{15} TPC)FeCl] emerged as efficient catalyst in selective hydroxylation of cyclohexane and adamantane at room temperature.



P. Venkatesan, J. Santhanalakshmi

Journal of Molecular Catalysis A: Chemical 326 (2010) 99

Synthesis, characterization and catalytic activity of trimetallic nanoparticles in the Suzuki C–C coupling reaction

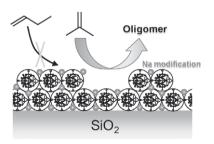
Pd containing trimetallic nanoparticles (Pdtnp) are synthesized using chemical method with cetyltrimethylammonium bromide (CTAB) as the capping agent. The particle sizes are characterized by HRTEM, and XRD measurements. The catalytic activities of Pdtnp are tested using Suzuki C–C coupling reaction. The product yield, reaction time and recyclability of the recovered catalysts are studied.

Jin Zhang, Mitsuru Kanno, Jiao Zhang, Ryuichiro Ohnishi, Kakeru Toriyabe, Hiromi Matsuhashi, Yuichi Kamiya

Journal of Molecular Catalysis A: Chemical 326 (2010) 107

Preferential oligomerization of isobutene in a mixture of isobutene and 1-butene over sodium-modified 12-tungstosilicic acid supported on silica

Na-modified ${\rm H_4SiW_{12}O_{40}/SiO_2}$ showed high selectivity (97%) for isobutene oligomerization in the preferential oligomerization of isobutene in an equimolar mixture of isobutene and 1-butene at 293 K.



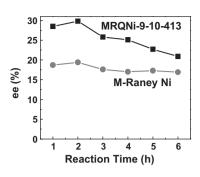
Contents ix

Zhiying Lou, Xueying Chen, Li Tian, Minghua Qiao, Kangnian Fan, Heyong He, Xiaoxin Zhang, Baoning Zong

Journal of Molecular Catalysis A: Chemical 326 (2010) 113

Preparation and characterization of the chirally modified rapidly quenched skeletal Ni catalyst for enantioselective hydrogenation of butanone to R-(-)-2-butanol

Chirally modified catalyst derived from the rapidly quenched skeletal Ni is more active and enantioselective than the similarly modified Raney Ni in the hydrogenation of butanone.

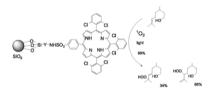


Sónia M. Ribeiro, Arménio C. Serra, A.M.d'A. Rocha Gonsalves

Journal of Molecular Catalysis A: Chemical 326 (2010) 121

Covalently immobilized porphyrins on silica modified structures as photooxidation catalysts

Covalent immobilization of a porphyrin on silica modified structures was achieved through a selective chlorosulphonation reaction. The resulting heterogeneous catalysts are active in singlet oxygen oxidation of α -terpinene and citronellol.

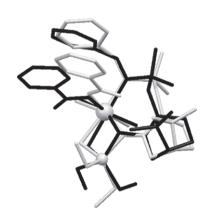


Anna Kozakiewicz, Małgorzata Ullrich, Mirosław Wełniak, Andrzej Wojtczak

Journal of Molecular Catalysis A: Chemical 326 (2010) 128

Synthesis, structure and activity of sulfonamides derived from (+)-camphor in the enantioselective addition of diethylzinc to benzaldehyde

New sulfonamide auxiliaries derived from (+)-camphor were used in the $\rm Et_2Zn$ addition to benzaldehyde (1–69% ee). 3D structures of Ti(IV) complexes were postulated, explaining observed % ee and product chirality.



Quentin Raffy, Rémy Ricoux, Elodie Sansiaume, Stéphanie Pethe, Jean-Pierre Mahy

Journal of Molecular Catalysis A: Chemical 326 (2010) 141

Corrigendum to "Coordination chemistry studies and peroxidase activity of a new artificial metalloenzyme built by the "Trojan horse" strategy" [J. Mol. Catal. A: Chem. 317 (1–2) (2009) 19–26]