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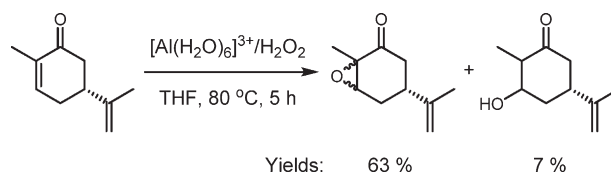
Articles

**Roberto Rinaldi, Heitor F.N. de Oliveira,
Herbert Schumann, Ulf Schuchardt**

Journal of Molecular Catalysis A: Chemical 307 (2009) 1

Homogeneously catalyzed epoxidation of α,β -unsaturated ketones using simple aluminum salts and aqueous H_2O_2 —Is it possible?

Simple aluminum salts can induce nucleophilicity to H_2O_2 allowing epoxidation at electron-deficient C=C bonds. Although the ionic pathway involving HOO^- species is prevailing towards α,β -unsaturated ketones, the radical pathway is revealed as the exclusive route followed in the reaction with diethylmaleate. In this reaction, radical addition of THF to diethylmaleate takes place selectively, affording 2-(THF)-derivatives with high yield.

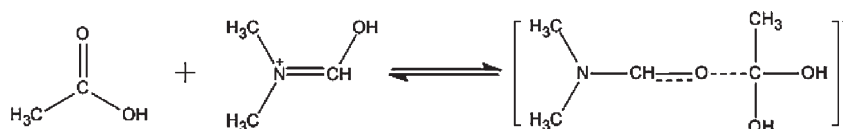


**Fei Xu, Hongyu Chen, Haibo Zhang, Xiaohai Zhou,
Gongzhen Cheng**

Journal of Molecular Catalysis A: Chemical 307 (2009) 9

Protophilic amide ionic liquid assisted esterification and catalysis mechanism

Brønsted acidic ionic liquids derived from protophilic amides can be used to catalyze esterification of alcohols by acetic acids under room temperature with Good conversion ratio and excellent reaction rate. An assumption about the possible mechanism is carried out by NMR.

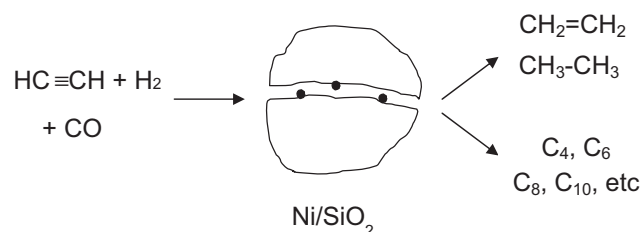


David L. Trimm, Irene O.Y. Liu, Noel W. Cant

Journal of Molecular Catalysis A: Chemical 307 (2009) 13

The effect of carbon monoxide on the oligomerization of acetylene in hydrogen over a Ni/SiO_2 catalyst

Carbon monoxide has two effects on the reaction of acetylene–hydrogen mixtures over a Ni/SiO_2 catalyst. Although it does not react, it improves acetylene conversion, initially and with time, and increases the selectivity to C_4 and higher products at the expense of ethylene and ethane by approximately 10%.

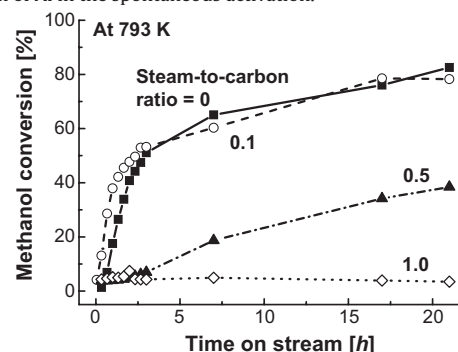


Jun Hyuk Jang, Ya Xu, Dong Hyun Chun, Masahiko Demura, Dang Moon Wee, Toshiyuki Hirano

Journal of Molecular Catalysis A: Chemical 307 (2009) 21

Effects of steam addition on the spontaneous activation in Ni₃Al foil catalysts during methanol decomposition

Steam addition was found to suppress the spontaneous activation which was characteristically observed in methanol decomposition over our newly discovered Ni₃Al foil catalysts. The results were related to the important role of selective oxidation/hydroxylation of Al in the spontaneous activation.

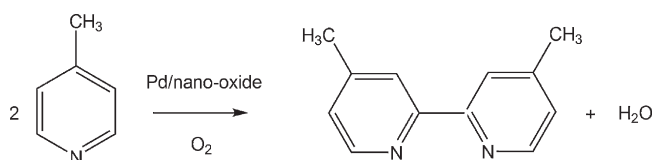


Luke M. Neal, Daniel Hernandez, Helena E. Hagelin-Weaver

Journal of Molecular Catalysis A: Chemical 307 (2009) 29

Effects of nanoparticle and porous metal oxide supports on the activity of palladium catalysts in the oxidative coupling of 4-methylpyridine

Palladium catalysts supported on several nanoparticle and porous metal oxides were prepared and characterized. Catalysts active in the oxidative coupling of 4-methylpyridine were supported on high surface area oxides or on oxides with strong palladium-support interactions.

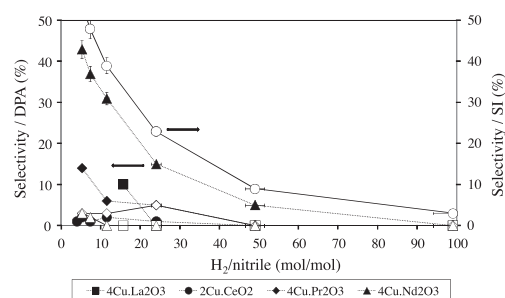


Joaquim Badalo Branco, Danielle Ballivet-Tkatchenko, António Pires de Matos

Journal of Molecular Catalysis A: Chemical 307 (2009) 37

Gas-phase hydrogenation of propionitrile on copper-lanthanide oxides

Copper-lanthanide oxide catalysts {2Cu-CeO₂ and 4Cu-Ln₂O₃ (Ln = La, Pr, Nd)} were active and selective for the gas-phase hydrogenation of propionitrile. The main product was the primary amine, *n*-propylamine. The catalysts were more selective than conventional copper impregnation catalysts, Cu (10 wt.%) on SiO₂, La₂O₃ or CeO₂, that produce significant quantities of dipropylamine.

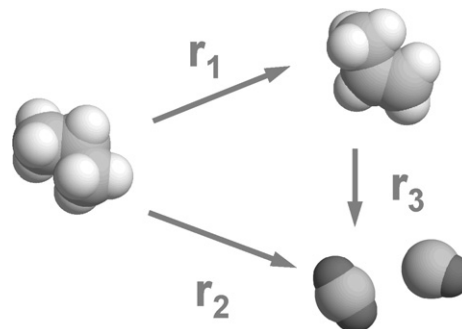


Arne Dinse, Sonia Khennache, Benjamin Frank, Christian Hess, Rita Herbert, Sabine Wrabetz, Robert Schlögl, Reinhard Schomäcker

Journal of Molecular Catalysis A: Chemical 307 (2009) 43

Oxidative dehydrogenation of propane on silica (SBA-15) supported vanadia catalysts: A kinetic investigation

A kinetic study was implemented to elucidate the reaction mechanism of oxidative dehydrogenation of propane (ODP) on a structurally well characterized silica (SBA-15) supported vanadia catalyst. Furthermore, calorimetric measurements were used to investigate the adsorption behaviour of propane on the catalyst surface. Reaction orders indicate a participation of propane and propene in the respective rate-determining steps of the particular partial reaction and a fast reoxidation of the reduced catalytic site. The results of the kinetic modelling and the adsorption experiments were used to calculate the real activation energies of the reaction.

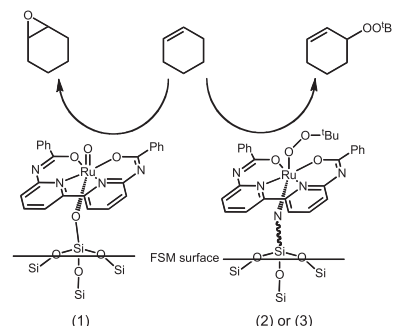


**Takeshi Okumura, Shinji Watanabe,
Takeyoshi Yagyu, Hideki Takagi,
Yoshiaki Fukushima, Hideki Masuda,
Koichiro Jitsukawa**

Journal of Molecular Catalysis A: Chemical 307 (2009) 51

Selectivity control of oxygen transfer reactions catalyzed by the ruthenium complexes with monodentate oxygen or nitrogen ligand bound to FSM

Ruthenium complexes immobilized into mesopore of FSM shows interesting catalytic activity for oxygen transfer reaction of cyclohexene using tert-butylhydroperoxide (TBHP) as an oxidant. The FSM-Ru catalyst (**1**) having oxygen donor gives 1,2-epoxycyclohexane selectively through stepwise addition of TBHP, but FSM-Aps-Ru (**2**) or FSM-Ims-Ru (**3**) having nitrogen donor gives 2-cyclohexen-1-yl tert-butyl peroxide mainly. This remarkable selectivity control in the oxygen transfer reaction is interpreted in terms of the *trans*-influence of the ruthenium complex with the axially coordinating monodentate ligand on the silica support.

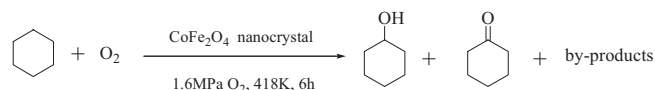


**Jinhui Tong, Lili Bo, Zhen Li, Ziqiang Lei,
Chungu Xia**

Journal of Molecular Catalysis A: Chemical 307 (2009) 58

Magnetic CoFe₂O₄ nanocrystal: A novel and efficient heterogeneous catalyst for aerobic oxidation of cyclohexane

Magnetic nanocrystalline spinel-type cobalt ferrite complex oxides were prepared at different molar ratios of Co^{II} to Fe^{III} and well characterized. These samples show high catalytic activities for heterogeneous oxidation of cyclohexane with molecular oxygen without any solvents or reductants. When pure CoFe₂O₄ was used as catalyst, 16.2% of cyclohexane conversion and 92.4% of selectivity for cyclohexanone and cyclohexanol were obtained. The catalyst could be easily separated by an external magnet and no obvious loss of activity was observed when it was reused in five consecutive runs.

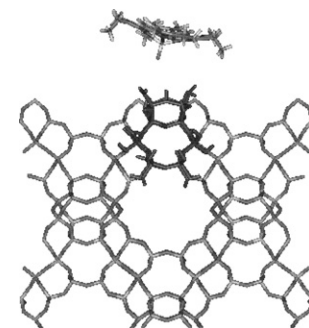


I.P. Zaragoza, R. Santamaria, R. Salcedo

Journal of Molecular Catalysis A: Chemical 307 (2009) 64

The interaction of vanadyl porphyrin with the HY zeolite surface

The interaction of vanadyl porphyrin with the HY zeolite surface. The shaded atoms of the zeolite, plus the atoms of the porphyrin, are taken into consideration in the molecular simulation. A larger portion than the zeolite model surface used in the simulations is sketched as an overview of the zeolite unit cell.

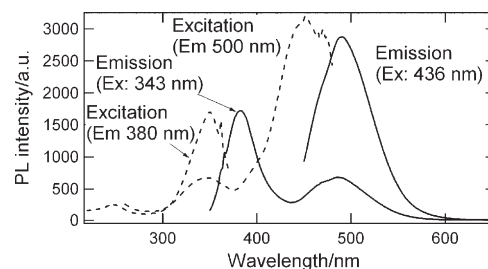


**Takeo Masuda, Tsunenori Watanabe,
Yuya Miyahara, Shinji Iwamoto, Hiroyoshi Kanai,
Masashi Inoue**

Journal of Molecular Catalysis A: Chemical 307 (2009) 71

Photoluminescence of propylene adsorbed on γ -Ga₂O₃-Al₂O₃ solid solutions in relation to their catalysis for CH₄-SCR of NO

When C₃H₆ adsorbed on γ -Ga₂O₃-Al₂O₃ solid solutions prepared by the solvothermal method was heated at 473 K and above, it discolored yellow. Its photoluminescence emission showed bands at 383 and 487 nm by the excitation with 343 nm light, and a band at 491 nm by 436 nm light. The emission intensity at 383 nm is related with the catalytic activity of γ -Ga₂O₃-Al₂O₃ for CH₄-SCR of NO.

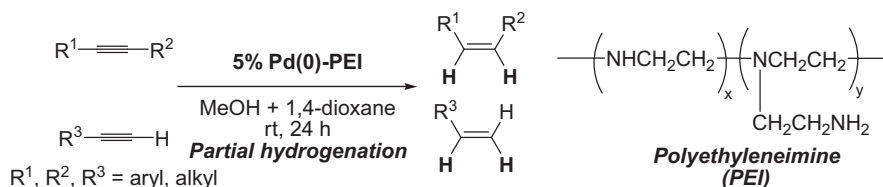


Shigeki Mori, Tomoyuki Ohkubo, Takashi Ikawa, Akira Kume, Tomohiro Maegawa, Yasunari Monguchi, Hironao Sajiki

Journal of Molecular Catalysis A: Chemical 307 (2009) 77

Pd(0)-polyethyleneimine complex as a partial hydrogenation catalyst of alkynes to alkenes

A Pd(0)-polyethyleneimine (PEI) complex was prepared by mixing Pd(OAc)₂ and PEI under H₂ atmosphere, and used as a catalyst for the partial hydrogenation of a variety of *mono*- and *di*-substituted alkynes producing the corresponding (*cis*-)alkenes with high selectivity. Moreover, the Pd(0)-PEI complex catalyzed the chemoselective hydrogenation of only *mono*-substituted alkynes with other reducible functionalities untouched.

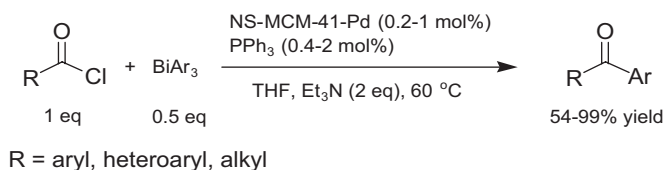


Jun-You Chen, Szu-Chien Chen, Yun-Ju Tang, Chung-Yuan Mou, Fu-Yu Tsai

Journal of Molecular Catalysis A: Chemical 307 (2009) 88

Coupling of acyl chlorides with triaryl bismuths catalyzed by palladium bipyridyl complex anchored on nanosized MCM-41: A recyclable and atom-efficient catalytic process for the synthesis of diaryl and alkyl aryl ketones

Palladium bipyridyl complex anchored on nanosized MCM-41 was used as a heterogeneous catalyst for the cross-coupling of acyl chlorides and triaryl bismuths. This catalyst could be recovered and re-used several times without significant loss of its catalytic activity.

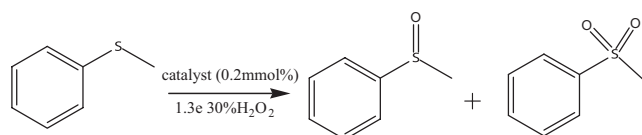


Fang Xie, Zaihui Fu, Sheng Zhong, Zhengpei Ye, Xiaoping Zhou, Fenglan Liu, Chunying Rong, Liqiu Mao, Dulin Yin

Journal of Molecular Catalysis A: Chemical 307 (2009) 93

Thioanisole oxidation with hydrogen peroxide catalyzed by hexadentate 8-quinolinolato manganese(III) complexes

Hexadentate 8-quinolinolato manganese(III) complexes (Q₃Mn^{III}) developed by us, with the help of NH₄OAc and HOAc, were found to efficiently catalyze the mild oxidation of thioanisole with aqueous hydrogen peroxide in environmentally benign acetone-water media.



Rogelio Charles, Rebeca González-Hernández, Elsa Morales, Javier Revilla, Luis E. Elizalde, Gregorio Cadenas, Odilia Pérez-Camacho, Scott Collins

Journal of Molecular Catalysis A: Chemical 307 (2009) 98

Novel supported catalysts for ethylene polymerization based on aluminohydride-zirconocene complexes

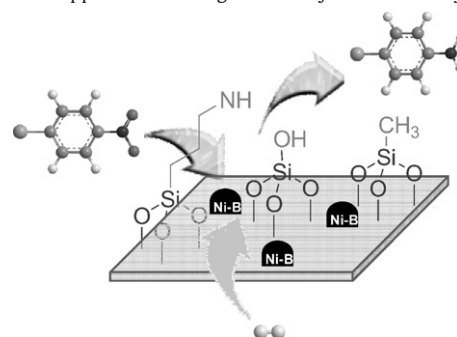
Active supported catalysts for ethylene polymerization are derived from reaction of zirconocene aluminohydride complexes with methylaluminoxane-treated silica. Depending on the method of activation, polymerization activity and polymer MW are significantly increased compared with the corresponding dichloride complexes.



Hui Li, Ye Xu, Haixia Yang, Fang Zhang, Hexing Li*Journal of Molecular Catalysis A: Chemical* 307 (2009) 105

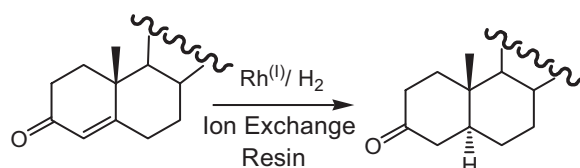
Ni-B amorphous alloy deposited on an aminopropyl and methyl co-functionalized SBA-15 as a highly active catalyst for chloronitrobenzene hydrogenation

SBA-15 type mesoporous silica co-functionalized with aminopropyl and methyl groups was synthesized through P123 directed co-condensation of tetraethoxysilane with aminopropyl and methyl triethoxysilanes. The Ni-B amorphous alloy catalyst deposited on such support showed higher activity and selectivity in liquid-phase hydrogenation of *p*-chloronitrobenzene owing to the synergetic promotions from both the aminopropyl and methyl groups.

**Rui M.D. Nunes, Tânia F. Fernandes, Glenda A. Carvalho, Eduardo N. dos Santos, Maria José S.M. Moreno, A.P. Piedade, Mariette M. Pereira***Journal of Molecular Catalysis A: Chemical* 307 (2009) 115

Recyclable immobilized rhodium catalysts in the diastereoselective hydrogenation of unsaturated steroids

A comparative study of the hydrogenation of unsaturated oxosteroids using immobilized rhodium catalysts onto ion exchange resins is described. These new immobilized catalysts show a high activity combined with easy product separation and catalyst reuse. This set of results makes the process here reported very attractive for performing the chemo, regio and diastereoselective hydrogenation of multifunctional steroid molecules.

**JinTang Guo, YaQin Ye, Shan Gao, YaKai Feng***Journal of Molecular Catalysis A: Chemical* 307 (2009) 121

Synthesis of polyketone catalyzed by Pd/C catalyst

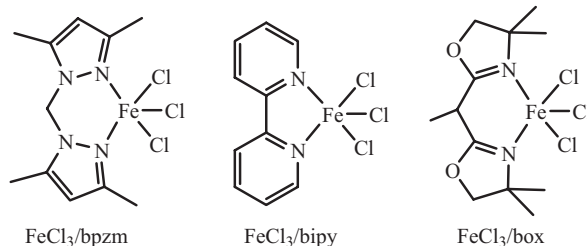
In the present work, polyketone (STCO) was successfully synthesized by use of carbon monoxide (CO) and styrene (ST) in the presence of Pd/C (5.4 wt%), bipyridine and *p*-toluenesulfonic acid. The final products were characterized by many methods. The effects of various reaction conditions were investigated in detail, and the reusability of Pd/C catalyst in the copolymerization of CO and ST was also probed.

Characterization method	reaction conditions	Final results
Infrared Spectroscopy (IR)	Pd/C catalyst usage	Pd/C catalyst can be reused for 12 times
Nuclear Magnetic Resonance (¹³ C NMR)	ligands	the highest catalytic activity is 1255.17 STCO/gPd·h
Elemental Analysis and Transmission Electron Microscopy (TEM)	<i>p</i> -toluenesulfonic acid	The molecular weights of the polyketone were <i>M_n</i> = 10700, <i>M_w</i> = 19079
Thermogravimetry (TG) and Differential Scanning Calorimetry (DSC)	reaction temperature	polydispersity index of the polyketone were <i>M_w</i> / <i>M_n</i> = 1.78
Gel Permeation Chromatography (GPC)	reaction time	Polyketone was synthesized successfully

Rossella Ferro, Stefano Milione, Tonino Caruso, Alfonso Grassi*Journal of Molecular Catalysis A: Chemical* 307 (2009) 128

Iron(III) complexes of bidentate nitrogen ligands as catalysts in reverse atom transfer radical polymerization of styrene

FeCl₃/bpzm, FeCl₃/bipy and FeCl₃/box have been tested in reverse ATRP of styrene. The comparative study of the electrochemical properties and of the formation constants of these adducts permitted to rationalize the higher control observed in the radical polymerization catalyzed by FeCl₃/box.

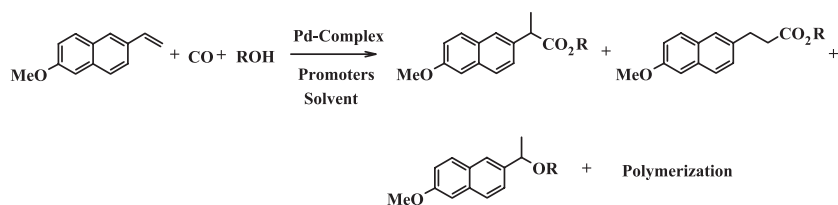


**Shashi B. Atla, Ashutosh A. Kelkar,
Raghunath V. Chaudhari**

Journal of Molecular Catalysis A: Chemical 307 (2009) 134

Hydroesterification of 2-vinyl-6-methoxynaphthalene using palladium complexes containing chelating nitrogen ligands

Palladium complexes containing chelating N[∞]O and N[∞]N were examined in the hydroesterification of 2-vinyl-6-methoxynaphthalene to the ester of naproxen. The acid and halide promoters were required to achieve high activity and selectivity. The effect of various reaction parameters was investigated. The turnover frequency using the complex Pd(acpy)(PPh₃)(OTs)₂ was found to be 42 h⁻¹.



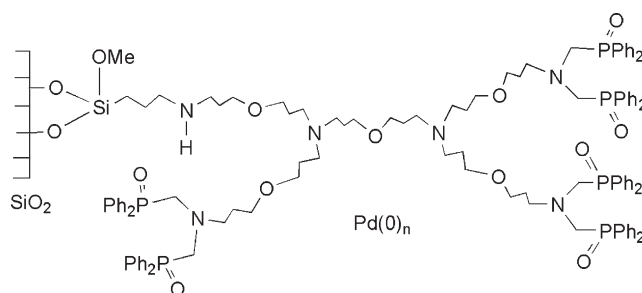
Hydroesterification of 2-vinyl-6-methoxynaphthalene

G. Jayamurugan, C.P. Umesh, N. Jayaraman

Journal of Molecular Catalysis A: Chemical 307 (2009) 142

Preparation and catalytic studies of palladium nanoparticles stabilized by dendritic phosphine ligand-functionalized silica

Dendritic phosphine functionalized silica was prepared and complexed with Pd(II). Subsequent formation of Pd(0) nanoparticle within the functionalized silica and the catalytic activities of the nanoparticles in a hydrogenation reaction are reported.

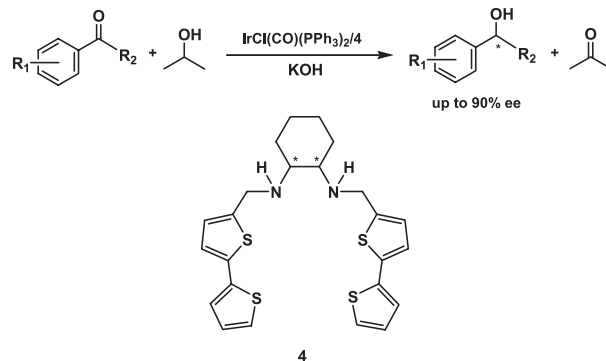


**Xue-Qin Zhang, Yan-Yun Li, Zhen-Rong Dong,
Wei-Yi Shen, Zhi-Bo Cheng, Jing-Xing Gao**

Journal of Molecular Catalysis A: Chemical 307 (2009) 149

Asymmetric transfer hydrogenation of aromatic ketones with chiral diamino-thiophene/iridium catalyst systems

The chiral diamino-bis(bithiophene) ligands were employed in the iridium(I)-catalyzed asymmetric transfer hydrogenation of aromatic ketones firstly, giving the corresponding optically secondary alcohols with high yield and up to 90% ee. The coordination environment of the diamino-thiophene ligands on the Ir atom was also investigated.



**Benjaram M. Reddy, Boningari Thirupathi,
Meghshyam K. Patil**

Journal of Molecular Catalysis A: Chemical 307 (2009) 154

Highly efficient promoted zirconia solid acid catalysts for synthesis of α -aminonitriles using trimethylsilyl cyanide

Highly efficient promoted zirconia solid acid catalysts for synthesis of α -aminonitriles using trimethylsilyl cyanide. Promoted zirconia catalysts were employed for multicomponent Strecker reaction of various aliphatic, aromatic and heterocyclic aldehydes or ketones with amine and TMS-CN in one step. These catalysts facilitated the reaction under mild conditions and provided good product yields.

