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Low-bromide containing MC catalyst for the autoxidation of *para*-xylene



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Synthesis of PVP-Ru amphiphilic microreactors with Ru nanocatalysts and their application in the fast hydrogenation of unsaturated compounds in aqueous media Fast hydrogenation of arenes, olefins and carbonyl compounds were successfully realized in the PVP-Ru microreactor system in aqueous media. The very high TOF values were contributed to the enrichment of poorly water-soluble organic substrates and hydrogen by hydrophobic microenvironment in microreactor in aqueous phase, and high active Ru nanoparticle catalysts



Nitin S. Nandurkar, Mayur J. Bhanushali, Malhari D. Bhor, Bhalchandra M. Bhanage

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 $Y(NO_3)_3$, GH_2O : A novel and reusable catalyst for one pot synthesis of 3,4-dihydropyrimidin-2(1H)ones under solvent-free conditions Yttrium(III) nitrate hexahydrate $[Y(NO_3)_3, 6H_2O]$ as a catalyst for organic reaction is described for the first time. The catalytic activity is demonstrated using Biginelli reaction as a model under solvent-free conditions. Excellent yields of dihydropyrmidinones are obtained at 70 °C within a short reaction time (10–50 min) and the catalyst is also recyclable. Other advantages over the classical method include greater substrate compatibility, faster reaction rates and easy workup procedures.



M. Alamé, M. Jahjah, S. Pellet-Rostaing, M. Lemaire, V. Meille, C. de Bellefon

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2,2'-Bis-[bis(4-substituted-phenyl)phosphino]-1,1'binaphthyl derivatives in Rh(I)-catalyzed hydrogenation of acetamidoacrylic acid derivatives: Electronic effects





Jhillu S. Yadav, Kamakolanu Uma Gayathri, Hissana Ather, Hafeez ur Rehman, Attaluri R. Prasad

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Utility of semicarbazones as ligands in newly made palladium complex for facile Suzuki homocoupling reaction of alkyl and aryl boronic acids



Majid M. Heravi, Leila Ranjbar, Fatemeh Derikvand, Fatemeh F. Bamoharram

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A modified and green Dakin–West reaction: An efficient and convenient method for a one-pot synthesis of β -acetamido carbonyl compounds

Δ

An efficient and improved procedure for the synthesis of β -acetamido carbonyl compounds is developed in the presence of trimethylsilyl chloride by a heteropolyacid catalyzed three-component coupling protocol.

$$\operatorname{ArCHO} + \operatorname{Ar'COCH}_{3} \text{ or } \operatorname{MeO}_{2}\operatorname{CCH}_{2}\operatorname{COCH}_{3} \xrightarrow{\text{heteropolyacid , CH}_{3}\operatorname{CO}} \xrightarrow{\operatorname{AcHN}} \xrightarrow{\operatorname{AcHN}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{Ar'}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{Ar'}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{Ar'}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{Ar'}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{Ar'}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{COOMe}} \xrightarrow{\operatorname{AcHN}} \operatorname{O}_{\operatorname{Ar'}} \xrightarrow{\operatorname{AcHN}} \operatorname{Ar'}$$

Hong-Chang Shi, Yong Li

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Formation of nitroxide radicals from secondary amines and peracids: A peroxyl radical oxidation pathway derived from electron spin resonance detection and density functional theory calculation Formation of nitroxide radicals from secondary amines and peracids is a peroxyl radical oxidation reaction with low activation barriers. By a calculation with DFT method at B3LYP/6-31G(d) level, it was found that the activation barriers of oxidizing pyrrolidine by the peroxyl radicals of peracetic acid and percarboximidic acid are 11.75 and 12.35 kcal/mol, respectively.



Jianmin Hao, Haiyang Cheng, Hongjun Wang, Shuxia Cai, Fengyu Zhao

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The selective oxidation of cyclohexane to cyclohexanol and cyclohexanone is an important chemical process and it has been paid more attentions recently. The present work demonstrated that the oxidation of cyclohexane could be promoted by stainless steel reactor wall and a new catalyst of quasi-crystalline alloy of $Ti_{45}Zr_{35}Ni_{17}Cu_3$ was active for the present reaction under the solvent-free conditions.

Oxidation of cyclohexane—A significant impact of stainless steel reactor wall





Dhanashri P. Sawant, A. Vinu, S.P. Mirajkar, F. Lefebvre, K. Ariga, S. Anandan, T. Mori, C. Nishimura, S.B. Halligudi

Nano-sized silicotungstic acid (STA) supported on zirconia embedded inside the mesoporous silicas such as SBA-15, MCM-41 and MCM-48 calcined at different temperatures were found to catalyze esterification of isoamyl alcohol (IAA) with acetic acid (AA). Fifteen weight percent STA/22.4 wt.% ZrO₂/SBA-15 calcined at 1123 K was the most active catalyst showed higher conversion and selectivity than in esterification of IAA by AA.

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Silicotungstic acid/zirconia immobilized on SBA-15 for esterifications



Where, R : CH₂CH₂CH(CH₃)₂



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Silica immobilized copper complexes: Efficient and reusable catalysts for *N*-arylation of N(H)-heterocycles and benzyl amines with aryl halides and arylboronic acids



Edimar DeOliveira, Alexandre G.S. Prado

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Ethylenediamine attached to silica as an efficient, reusable nanocatalyst for the addition of nitromethane to cyclopentenone Solid base nanocatalyst was developed and was applied and reused in the addition of nitromethane to cyclopentenone in equimolar conditions.



Dong Hyun Kim, Ueon Sang Shin, Choong Eui Song

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Oxidatively pure chiral (salen)Co(III)-X complexes *in situ* prepared by Lewis acid-promoted electron transfer from chiral (salen)Co(II) to oxygen: Their application in the hydrolytic kinetic resolution of terminal epoxides The Lewis acid (MX_3)-promoted oxidation of catalytically inactive chiral (salen)Co(II) afforded neither the mononuclear nor dinuclear heterobimetallic (salen)Co complexes as reported in the literatures, but rather selectively the Jacobsen's complexes, chiral (salen)Co(III)-X.



Babak Karimi, Maryam Khalkhali

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Silica functionalized sulfonic acid as a recyclable interphase catalyst for chemoselective thioacetalization of carbonyl compounds in water



Piero Frediani, Paolo Mariani, Luca Rosi, Marco Frediani, Alessandro Comucci

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One-pot syntheses of alcohols from olefins through Co/Ru tandem catalysis



The one-pot syntheses of primary alcohols from olefin through a tandem catalytic system $(Co_2(CO)_g \text{ for})$

hydroformylation and [Ru(CO)₂(PPh₃)X₂]₂ (X: Cl, Br, I) for hydrogenation) has been reached with very

Venkata Jaganmohan Reddy, Joanne Muriithi, M. Venkat Ram Reddy Novel *N*-boronomethyltrialkylammonium salts have been synthesized and utilized as catalysts for selective acetylation of primary alcohols and aldehydes.

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Novel quaternary ammoniumboronate salts as selective acylation catalysts



Hancheng Zhou, Feng Shi, Xiong Tian, Qinghua Zhang, Youquan Deng

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Synthesis of carbamates from aliphatic amines and dimethyl carbonate catalyzed by acid functional ionic liquids





Mingzhong Cai, Qiuhua Xu, Yixiang Huang

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Heterogeneous Suzuki reaction catalyzed by MCM-41-supported sulfur palladium(0) complex The MCM-41-supported sulfur palladium(0) complex has been synthesized from 3-(2-cyanoethylsulfanyl)propyltriethoxysilane via immobilization on MCM-41, followed by reacting with palladium chloride, and then the reduction with hydrazine hydrate. This complex is a highly active catalyst for the heterogeneous Suzuki reaction affording a variety of biaryls in high to excellent yields.



Kourosh Malek, Can Li, Rutger A. van Santen

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New theoretical insights into epoxidation of alkenes by immobilized Mn-salen complexes in mesopores: Effects of substrate, linker and confinement We performed calculations based on density functional theory in combination with molecular mechanics methodologies to investigate the origin of enantioselectivity in the epoxidation reaction of *cis*- and *trans*-methylstyrene, catalyzed by immobilized Mn-salen in MCM-41 channels. Our calculations provide new insights into the importance of electronic and steric effects of the salen ligand and substrates and the interplay with the immobilizing linker and MCM-41 confinement.



Yosslen Aray, Jesús Rodríguez, Alba Beatriz Vidal, Santiago Coll

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Nature of the NiMoS catalyst edge sites: An atom in molecules theory and electrostatic potential studies

The nature of the active sites on the NiMoS catalyst was explored using the combination of the atoms in molecules theory and an electrostatic potential based methodology. The active sites on the catalyst surface were localized visualizing the basin of the outermost atoms of the surface. Direct visualization (see picture at the left) of the interatomic metal–sulfur surface (white structures) defining the basin of the outermost atoms of the studied NiMoS edge models has shown that the Mo atoms are practically covered by the outermost S atoms (yellow spheres) while the promoter Ni (blue spheres) are the most accessible metal atoms to the exterior of the edges. Electrostatic potential mapping on the atomic border exposed to the exterior of the edge (picture at the right) has shown that the most acidity sites (red zones) are located at very small regions

(highlighted by black ellipses) at the Mo atoms on the Mo edges. However, the accesses to these sites are very impeded by the outermost S atoms. Adsorption of a molecule containing the pollutant atoms strongly depends on two factors: the Lewis acidity of the site and the repulsive interaction of the incoming molecule with sulfur atoms impeding the free access to the site. In this sense, the main role of the promoter is to produce uncovered Lewis acid sites.



Sami Habib, Petra Salamé, Franck Launay, Virginie Semmer-Herledan, Olivier Marie, Wei Zhao, Nataša Novak Tušar, Antoine Gédéon

Journal of Molecular Catalysis A: Chemical 271 (2007) 117

Investigation of the catalytic activity of extracted and smoothly calcined arenesulfonic modified SBA-15 materials FTIR studies showed that arenesulfonic modified SBA-15 solids display a good thermal stability between 200 and 400 °C. These results were confirmed by the thermogravimetric analyses of the calcined materials, i.e. EC-200 and EC-400. Both the extracted (E) and smoothly calcined solids (EC-200) exhibited high activities in the liquid phase condensation of 2-methylfuran with acetone and in the decomposition of cumene hydroperoxide into phenol.



Fatemeh F. Bamoharram, Majid M. Heravi, Mina Roshani, Manouchehr Jahangir, Ali Gharib

Catalytic activity of recyclable Preyssler acid, H_{14} - P_5 and its different forms such as H_{14} - P_5 Mo and H_{14} - P_5 /SiO₂ have been investigated, in liquid phase in the presence of hydrogen peroxide. A systematic study has been made to find the effect of catalyst type, the molar ratio of alcohol to hydrogen peroxide, temperature and the duration of reaction on the synthesis of the ester. All the catalysts have been found to be active and exhibit 100% selectivity and recyclable.

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Effective direct esterification of butanol by ecofriendly Preyssler catalyst, $[NaP_5W_{30}O_{110}]^{14-}$

 $CH_{3}CH_{2}CH_{2}CH_{2}OH \xleftarrow{\text{catalyst/H}_{2}O_{2},C_{2}H_{4}Cl_{2}} \\CH_{3}CH_{2}CH_{2}COOCH_{2}CH_{2}CH_{2}CH_{3}+H_{2}O \\Catalyst: H_{14}-P_{5}, H_{14}-P_{5}Mo. H_{14}-P_{5}/SiO_{2}$

Biswanath Das, Keetha Laxminarayana, B. Ravikanth

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Application of heterogeneous catalysts for an efficient synthesis of β -keto enol ethers



Osman Dayan, Bekir Çetinkaya

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Mono- and binuclear ruthenium(II) complexes containing pyridine-2,6-diimine (Pydim) ligands: Synthesis, characterization and catalytic activity in the transfer hydrogenation of acetophenone Pydim-Ru(II) complexes have been employed as catalysts for the transfer hydrogenation of acetophenone. Significant differences in reactivity were observed according to the type of pydim ligand.



Akbar Heydari, Afsaneh Arefi, Samad Khaksar, Roohollah Kazem Shiroodi

Commercially available guanidine hydrochloride (GuHCl) has been found to be a highly efficient catalyst for the Strecker reaction.

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Guanidine hydrochloride: An active and simple catalyst for Strecker type reaction



Mireia Rodriguez-Zubiri, Stephane Anguille, Jean-Jacques Brunet

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Intermolecular hydroamination of non-activated alkenes catalyzed by Pt(II) or Pt(IV)-*n*-Bu₄PX (X = Cl, Br, I) systems: Key effect of the halide anion



Ashok Kumar Singh, Jaya Srivastava, Shahla Rahmani

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Mechanistic studies of oxidation of D-arabinose and D-mannose by acidic solution of *N*-bromoacetamide in presence of chloro-complex of Ru(III) as homogeneous catalyst

Kinetics and mechanism of Ru(III)-catalyzed oxidation of D-arabinose and D-mannose by acidic solution of N-bromoacetamide have been studied at 40°C. HOBr as the reactive species of NBA and RuCl₃(H₂O)₂OH]⁻ as the reactive species of Ru(III) chloride in acidic medium have been proposed for the oxidation of aforesaid reducing sugars. The size of the activated complex (d_{AB}) and various activation parameters have been calculated. On the basis of spectrophotometric and kinetic analysis of the data, a most probable reaction scheme, common for both arabinose and mannose, has been proposed. The formation of most unstable activated complex, by the interaction of two oppositely charged species, i.e. [Hg N OBr]⁺ and [RuCl₃:S·(H₂O) OH]⁻ is supported by the observed positive entropy of activation.

J.S. Yadav, B.V. Subba Reddy, K. Premalatha, M.S.R. Murty

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Bi(OTf)₃-catalyzed condensation of 2,2-DMP with aromatic amines: A rapid synthesis of 2,2,4-trimethyl-1,2-dihydroquinolines



K.S. Anisia, A. Kumar

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Oxidation of cyclohexane with molecular oxygen in presence of characterized macrocyclic heteronuclear FeCu complex catalyst ionically bonded to zirconium pillared montmorillonite clay Heteronuclear macrocyclic complex of iron and copper, $FeCuL(NO_3)_24H_2O$ [L = $(CH_3C_6H_2CH_2O(CH_2)_3N)_2$] was synthesized and a general scheme for bonding the complexes ionically on acidified montmorillonite clay was evolved. The kinetic analysis by genetic algorithm shows the catalysts to be highly efficient, specific to forming cyclohexanone.



P.J. Baricelli, Dayanna Baricelli, E. Lujano, L.G. Melean, M. Borusiak, Francisco López-Linares, Luis Jhonatan Bastidas, Merlín Rosales

The synthesis and characterization of the water-soluble complex $HRh(CO)(TPPMS)_3$ is described. This complex was obtained in situ and by ligand exchange procedures. These analyses confirmed that the rhodium complex has a trigonal prismatic arrangement. The complex was used as a catalytic precursor for the aqueous biphasic hydrogenation of several olefins and olefins mixtures. The observed catalytic activity was styrene > 1-hexene > cyclohexene > 2,3-dimethyl-1-butene. The catalyst was shown to be resistant to sulfur poisons.

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Catalytic hydrogenation of olefins and their mixtures using HRh(CO)(TPPMS)₃ complex in an aqueous biphasic medium



Anibal Sierraalta, Rafael Añez, Elena Ehrmann

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ONIOM study of Ga/SAPO-11 catalyst: Species formation and reactivity



Andrea Schmidt, Reinhard Schomäcker

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Partial hydrogenation of sunflower oil in a membrane reactor Partial hydrogenation of sunflower oil was carried out in a membrane reactor in pore-flow-through mode in n-heptane as solvent. Hydrogenation experiments were performed at different temperatures, hydrogen pressures and metals as catalysts. The stearic acid content at an iodine value (IV) of about 80 was 10–15% in the membrane reactor, 45% in the slurry reactor, respectively. The selectivity for the monoene fatty acids could be improved by decreasing hydrogen pressure.



Contents

Jiahui Huang, Ge Tian, Hongsu Wang, Ling Xu, Qiubin Kan

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Large-pore cubic Ia-3d mesoporous silicas: Synthesis, modification and catalytic applications Large-pore cubic Ia-3d mesoporous silicas were synthesized by co-condensation of tetraethoxysilane and phenyltriethoxysilane under acidic conditions. In the synthesis, the amount of PTES added and the prehydrolysis of PTES prior to TEOS were very vital for the formation of the ordered Ia-3d structure. By further modifications, sulfonic acid sites and amino groups were respectively introduced into the channels of Ia-3d mesoporous materials. These Ia-3d mesoporous acid and base catalysts were found to be very efficient in the synthesis of Bisphenol A and flavanone, respectively.



Ji-Jun Zou, Zhongqiang Xiong, Li Wang, Xiangwen Zhang, Zhentao Mi

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Preparation of $Pd-B/\gamma-Al_2O_3$ amorphous catalyst for the hydrogenation of tricyclopentadiene

The preparation conditions have significant effect on the properties and activity of Pd-B/ γ -Al₂O₃ amorphous catalyst. The amorphous catalyst is thermally stable at temperature below 150 °C and shows stronger H₂-adsorption capacity than crystallized metals with comparative surface. It exhibits high activity for the hydrogenation of tricyclopentadiene (TCPD) and a linear relationship is observed between the activity and amount of H₂-adsorption.



Ümit Bilge Demirci, François Garin

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Kinetic study of *n*-heptane conversion on palladium or iridium supported on sulphated zirconia

The metal-proton adduct site (below) explains the particular behaviour of Ir or Pd supported on sulphated zirconia for *n*-heptane conversion. The kinetic data suggest a transition from a bifunctional catalysis to an acid catalysis with increasing hydrogen pressure and/or reaction temperature.

 $[H-(Ir_m)(H^+)_x]^{x^+}$ \uparrow Metal-proton adduct \downarrow

 $[H-(Pd_n)(H^+)_y]^{y+1}$

Antonio Arques, Ana M. Amat, Lucas Santos-Juanes, Rosa F. Vercher, María L. Marín, Miguel A. Miranda

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Sepiolites as supporting material for organic sensitisers employed in heterogeneous solar photocatalysis



Contents

Yolanda Pérez, Damián Pérez Quintanilla, Mariano Fajardo, Isabel Sierra, Isabel del Hierro

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Immobilization of titanium chiral alkoxides on SBA-15 and modelling the active sites of heterogeneous catalyst using titanium silsesquioxane complexes

A molecular precursor approach involving simple grafting procedures was used to produce site isolated titanium-supported epoxidation catalysts. Organotitanium complexes bearing chiral groups react with the remaining hydroxyl groups of SBA-15 after silanization with Me₃SiCl yielding mostly isolated Ti(IV) sites, as evidenced by DRUV-vis. In addition, silsesquioxane derivatives have been synthesized in order to compare the different homogeneous and heterogenous systems mentioned above in the asymmetric epoxidation of cinnamyl alcohol to evaluate their catalytic activity and enantioselectivity.



A.M. Venezia, R. Murania, G. Pantaleo, G. Deganello

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Nature of cobalt active species in hydrodesulfurization catalysts: Combined support and preparation method effects

Co based catalysts for HDS were prepared by wet impregnation and by precipitation in the presence of sodium carbonate. The influence of different support and of the different preparation methods was related to the formation of Co_3O_4 . Increased cobalt reducibility and cobalt dispersion accounted for the observed differences.



Xuebing Zhao, Ting Zhang, Yujie Zhou, Dehua Liu

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Preparation of peracetic acid from hydrogen peroxide Part I: Kinetics for peracetic acid synthesis and hydrolysis

A homogeneous kinetic model for sulfuric acid-catalyzed preparation of peracetic acid by the reaction of hydrogen peroxide and acetic acid in the liquid phase was developed. The kinetic constants were determined by fitting the experimental data. Sufficient accuracy was obtained by using the model to describe the concentrations of peracetic acid in the reaction system, as shown in the following figure.



Veeresh Seregar, T.M. Veeresh, Sharanappa T. Nandibewoor

The kinetics of oxidation of L-leucine by diperiodatoargentate(III) (DPA) in the presence of micro amounts of osmium(VIII) in alkaline medium has been studied. The active species of DPA is found to be $[Ag(H_2IO_6)(H_2O)_2]$ and that of osmium(VIII) to be $[OsO_4(OH)_2]^{2-1}$ in alkaline medium. Journal of Molecular Catalysis A: Chemical 271

(2007) 253Osmium(VIII) catalysed oxidation of L-leucine by a

new oxidant, diperiodatoargentate(III) in aqueous alkaline medium

$$R - C H - COO^{-} + 2[Ag(H_{2}IO_{6})(H_{2}O)_{2}] + 4OH^{-} \xrightarrow{Os(VIII)} R - C OOH + 2Ag(I) + NH_{3} (1)$$

$$H_{2} + HCO_{3}^{-} + 2H_{2}IO_{6}^{3-} + 5H_{2}O$$
Where $R = -CH_{2}-CH < CH_{3} - CH_{3}$

Ji Chul Jung, Howon Lee, Heesoo Kim, Young-Min Chung, Tae Jin Kim, Seong Jun Lee, Seung-Hoon Oh, Yong Seung Kim, In Kyu Song

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A synergistic effect of α -Bi₂Mo₃O₁₂ and γ -Bi₂MoO₆ catalysts in the oxidative dehydrogenation of C₄ raffinate-3 to 1,3-butadiene

A series of mixed catalysts composed of α -Bi₂Mo₃O₁₂ and γ -Bi₂MoO₆ were prepared by a mechanical mixing method to investigate any synergistic effects of these two catalysts in the oxidative dehydrogenation of C₄ raffinate-3 to 1,3-butadine. The conversion of *n*-butene and the yield for 1,3-butadine over the mixed catalysts showed volcano-shaped curves with respect to γ -Bi₂MoO₆ content due to the synergistic effect of the α -Bi₂MoO₆ catalysts.



J.S. Yadav, B.V. Subba Reddy, P. Murali Krishna Reddy, Uttam Dash, Manoj K. Gupta

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Indium(III) bromide catalyzed cleavage of cyclic and acyclic ethers: An efficient and practical ring opening reaction



Debabrata Chatterjee, Susan Basak, Jacques Muzart

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Asymmetric epoxidation of alkenes with aqueous *t*-BuOOH catalyzed by novel chiral complexes of chromium(III) containing tridentate Schiff-base ligands

Mixed-ligand chromium catalyst containing tridentate sugar-based chiral ligand and bipyridine effect asymmetric induction in epoxidation of styrene using aqueous *t*-BuOOH as a terminal oxidant.



Holger B. Friedrich, Vikash Gokul

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A comparative study of the ruthenium(VI)dioxocarboxylato salts, $[PPh_4][RuO_2(OCOR)Cl_2] \ (R=CH_3, CF_3, C_6H_5, C_6F_5, C_5H_{11}),$ in the oxidation of alcohols

The compounds $[PPh_4][Ru(O)_2(OCOR)Cl_2]$ (R = CH₃ 1a, CF₃ 1b, C₆H₅ 1c, C₆F₅ 1d, C₅H₁₁ 1e) were prepared and fully characterised. They were compared in the selective stoichiometric and catalytic oxidation of a number of alcohols to their corresponding carbonyl compounds, with a wide range of co-oxidants.



Yuan Zhao, Jie-Sheng Tian, Xin-Hua Qi, Zhe-Nan Han, Yuan-Yi Zhuang, Liang-Nian He

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Quaternary ammonium salt-functionalized chitosan: An easily recyclable catalyst for efficient synthesis of cyclic carbonates from epoxides and carbon dioxide. A quaternary ammonium salt covalently bound to chitosan (a functionalized biopolymer) is reported as an efficient and recyclable single-component catalyst for the synthesis of propylene carbonate from propylene oxide and CO_2 without any organic solvent or co-catalyst. Notably, this environmental benign and cost-effective process has great potential to be applied in various continuous flow reactors in industry.

