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JOURNAL OF MOLECULAR CATALYSIS A: CHEMICAL

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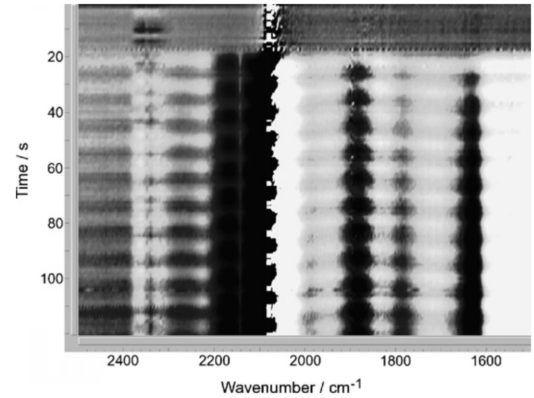

Cristina N. Nenu, Philippe Bodart, Bert M. Weckhuysen

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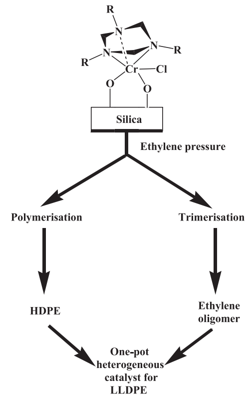
Turning a Cr-based heterogeneous ethylene polymerisation catalyst into a selective ethylene trimerisation catalyst

A single-site heterogeneous Cr-based catalyst can interchange trimerisation activity with polymerisation activity as a function of ethylene pressure. At low ethylene pressures, branched oligomers of ethylene are obtained and HDPE-type polymers are obtained at high ethylene pressures. At moderate pressures, this system can be considered a one-pot heterogeneous catalyst for production of LLDPE-type polymers.



Biswanath Das, Ponnaboina Thirupathi

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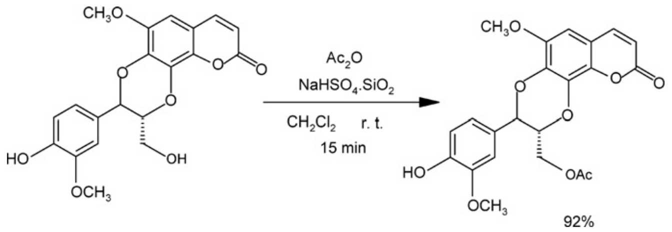
A highly selective and efficient acetylation of alcohols and amines with acetic anhydride using $NaHSO_4 \cdot SiO_2$ as a heterogeneous catalyst



doi:10.1016/S1381-1169(07)00098-2

Biswanath Das, Katta Venkateswarlu,
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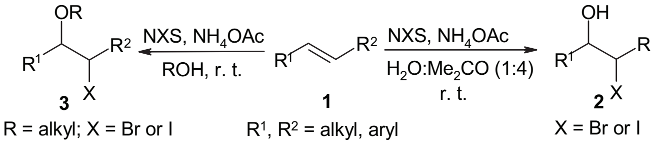
Ammonium acetate catalyzed improved method for the regioselective conversion of olefins into halohydrins and haloethers at room temperature



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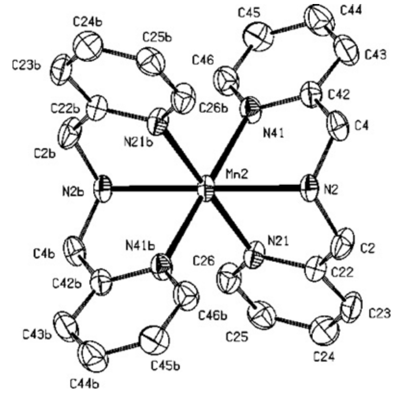
Synthesis, structural characterization, catalase-like function and epoxidation activity of a mononuclear manganese(II) complex

A manganese(II) complex using the tridentate ligand bpma (*N*,*N*-bis(2-pyridylmethyl)amine) $[Mn(bpma)_2](ClO_4)_2$ was prepared. The structure shows two different conformers with pseudo-octahedral geometry. The synthesized manganese complex displays efficiency in disproportion reactions of hydrogen peroxide producing water and dioxygen in catalase-like activity. The ability of the complex in an epoxidation reaction in homogeneous and heterogeneous media was also studied.



M. Radha Kishan, V. Radha Rani, P. Sita Devi,
S.J. Kulkarni, K.V. Raghavan

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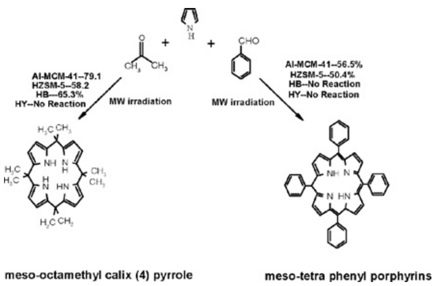
A novel zeolite based stationary phases for in situ synthesis and evaluation of porphyrins and calix (4) pyrroles

The present study, using a novel concept of reaction cum separation on a single plate for efficient evaluation of porphyrins and calix (4) pyrroles by in situ synthesis from pyrrole with aromatic aldehydes and ketones, respectively, over zeolite based molecular sieve catalysts as sorbents in thin layer chromatography (TLC) was accomplished in one step with microwave heating. The design and methodology of this glass-backed zeolite coated TLC, which acted as a micro reactor as well as separator for the in situ synthesis and evaluation of macrocycles is described.



Amit Saxena, Ajeet Kumar, Subho Mozumdar

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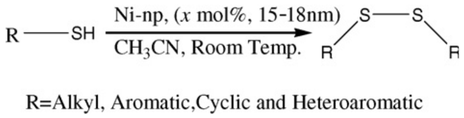
Ni-nanoparticles: An efficient green catalyst for chemo-selective oxidative coupling of thiols

A novel method for oxidative coupling of thiols to their corresponding disulfides using Ni-nanoparticles is described. Ni-nanoparticles act as novel and selective catalyst, which efficiently reduces the reaction time, increases the product yield without producing over oxidized products and perform under air atmosphere.



Kyung Won La, Ji Chul Jung, Heesoo Kim, Sung-Hyeon Baeck, In Kyu Song

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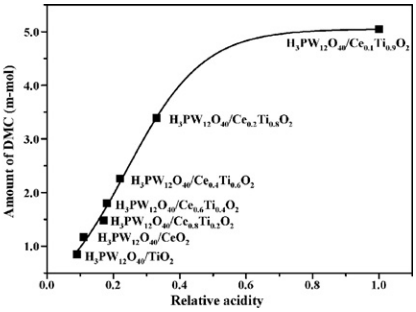
Effect of acid–base properties of $H_3PW_{12}O_{40}/Ce_xTi_{1-x}O_2$ catalysts on the direct synthesis of dimethyl carbonate from methanol and carbon dioxide: A TPD study of $H_3PW_{12}O_{40}/Ce_xTi_{1-x}O_2$ catalysts

$H_3PW_{12}O_{40}/Ce_xTi_{1-x}O_2$ catalysts prepared by a sol–gel method were applied to the direct synthesis of dimethyl carbonate (DMC) from methanol and carbon dioxide. The catalytic activity of $H_3PW_{12}O_{40}/Ce_xTi_{1-x}O_2$ increased with increasing acidity and with increasing basicity of the catalyst.



Guofang Zuo, Huiqing Yuan, Jiandong Yang, Ruixue Zuo, Xiaoquan Lu

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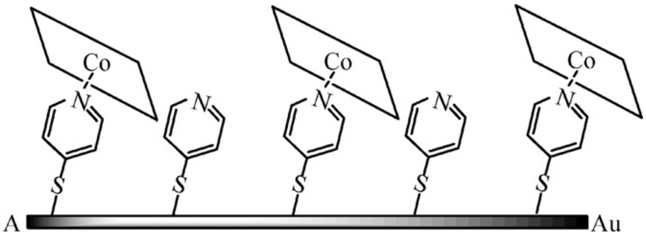
Study of orientation mode of cobalt-porphyrin on the surface of gold electrode by electrocatalytic dioxygen reduction

In this paper we prepared three cobalt-porphyrin-overlayered SAMs on gold and combined imidazole axial with Co-TPP to investigate the orientation mode of porphyrin ring by catalytic oxygen reduction. Porphyrin molecules of Co-TPP on 4MPY/SAMs was little parallelly tilted oriented to the gold surface. The porphyrin ring of Co-TPP on Co-TMPP/SAMs was oriented parallelly and on Co-ATP-MPA/SAMs was little perpendicularly tilted oriented on the electrode surface, respectively.



Srinivas Kantevari, Rajashaker Bantu, Lingaiah Nagarapu

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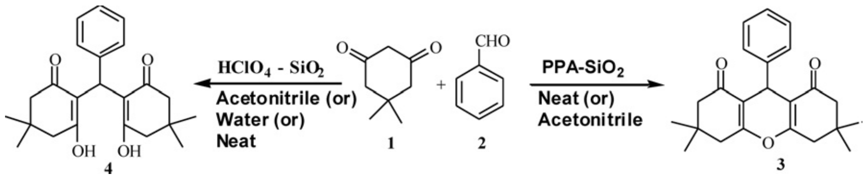
$HClO_4–SiO_2$ and PPA–SiO_2 catalyzed efficient one-pot Knoevenagel condensation, Michael addition and cyclo-dehydration of dimedone and aldehydes in acetonitrile, aqueous and solvent free conditions: Scope and limitations



David Raju Burri, Kwang-Min Choi, Sang-Cheol Han, Abhishek Burri, Sang-Eon Park

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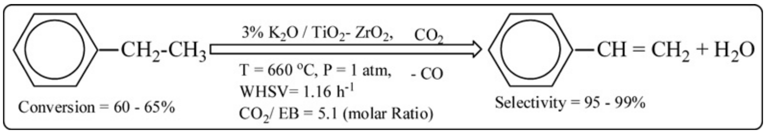
Selective conversion of ethylbenzene into styrene over K_2O/TiO_2-ZrO_2 catalysts: Unified effects of K_2O and CO_2



C. Paun, J. Barklie, P. Goodrich,
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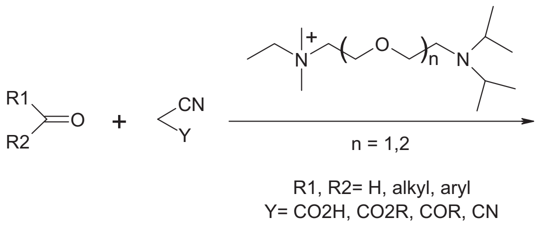
Supported and liquid phase task specific ionic liquids for base catalysed Knoevenagel reactions



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D.V. Korchagina, E.A. Paukshtis, E.M. Moroz,
K.P. Volcho, V.A. Barkhash, N.F. Salakhutdinov

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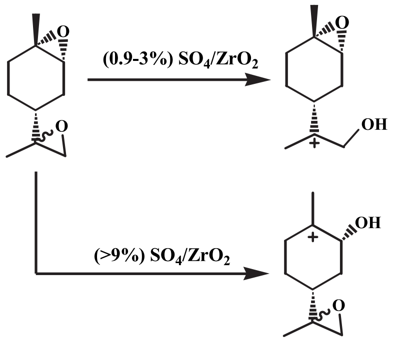
Effects of the properties of SO_4/ZrO_2 solid catalysts on the products of transformation and reaction mechanism of *R*-(+)-limonene diepoxides

The mechanism of diepoxide transformations at room temperature may be changed by varying the type and amount of acid centers on SO_4/ZrO_2. At a sulfation level of 0.9–3%, the products of the initial cleavage of the 8,9-epoxy group of limonene diepoxides were dominant. When the sulfo group content increased to more than 9%, the key transformations were those that started with cleavage of the 1,2-epoxy group.



Biswanath Das, Kongara Damodar,
Nikhil Chowdhury

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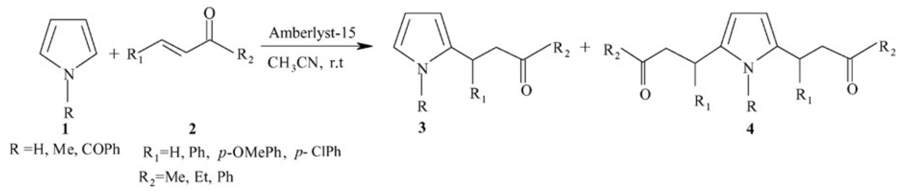
Amberlyst-15: A mild, efficient and reusable heterogeneous catalyst for Michael addition of pyrroles to α,β-unsaturated ketones



Suyun Jie, Shu Zhang, Wen-Hua Sun,
Xiaofei Kuang, Tianfu Liu, Jianping Guo

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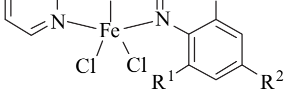
Iron(II) complexes ligated by 2-imino-1,10-phenanthrolines: Preparation and catalytic behavior toward ethylene oligomerization

A series of *N*,*N*,*N*-tridentate iron (II) complexes bearing 2-imino-1,10-phenanthrolines was synthesized and characterized. Activated with methylaluminoxane (MAO) or modified methylaluminoxane (MMAO), those iron complexes were found to be highly active catalysts for ethylene reactivity with high selectivity for α-olefins. The influences of the reaction parameters were examined for the inherent regularity of catalytic behavior.



Jianhua Liu, Hugjiltu Wu, Liwen Xu, Jing Chen, Chungu Xia

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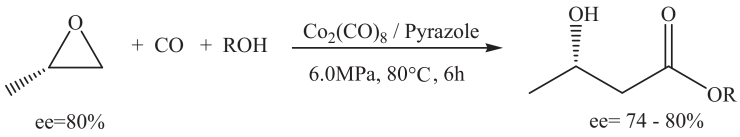
A novel and highly effective catalytic system for alkoxycarbonylation of (*S*)-propylene oxide

Methyl (*S*)-β-hydroxybutyrate was produced in high yield from the methoxycarbonylation of (*S*)-propylene oxide ((*S*)-PO) using a catalytic system consisting of dicobalt octacarbonyl [$Co_2(CO)_8$] and pyrazole in methanol. The effects of different additives, temperature and CO pressure were investigated. The reaction was greatly influenced by the variation of temperature, both the conversion of (*S*)-PO and the selectivity of methyl (*S*)-β-hydroxybutyrate decreased with increasing temperature (above 80 °C). Nevertheless, the enantiomeric excess (ee) of methyl (*S*)-β-hydroxybutyrate is independent of the parameters of reaction temperature, no racemization reaction takes place even the reaction temperature reaches 150 °C. The reaction can be extended to synthesize different β-hydroxybutyrates. The reaction will have a bright future in an industrial scale.



R=CH_3, C_2H_5, n-Pr, i-Pr, n-Bu, $PhCH_2$

Qiang Liu, Huamei Chen, Hai Lin, Huakuan Lin

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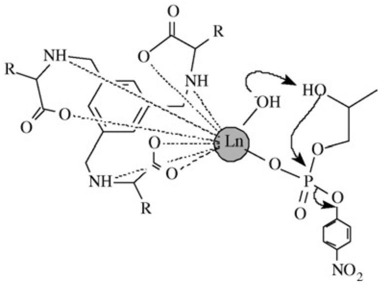
Study on kinetics and mechanism of mononuclear rare earth metal complexes in promoting the hydrolysis of 2-hydroxy-propyl-*p*-nitrophenyl phosphate (HPNP)

Kinetics and mechanism of promoted hydrolysis of 2-hydroxy-propyl-*p*-nitrophenyl phosphate (HPNP) by complexes of tripodal ligands L1 and L2 with La(III) and Gd(III).



Isabelle Kondolff, Henri Doucet, Maurice Santelli

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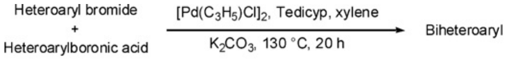
Synthesis of biheteroaryl derivatives by tetraphosphine/palladium-catalysed Suzuki coupling of heteroaryl bromides with heteroarylboronic acids

The Tedicyp–palladium system proves to be an efficient catalyst for the coupling of heteroarylboronic acids with heteroaryl bromides. Since the electronic properties of heteroarylboronic acids appears to have a minor influence on the reactions rates, their coordinative/poisoning properties to palladium seems to have a decisive influence. On the other hand, the electronic properties of the heteroaryl bromide often have an important effect on the yields and rates of the reactions.



Heteroaryl = thiophene, benzothiophene, furane, benzofurane, pyridine, quinoline, pyrimidine

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Marcin Konkol, Harry Schmidt, Dirk Steinborn

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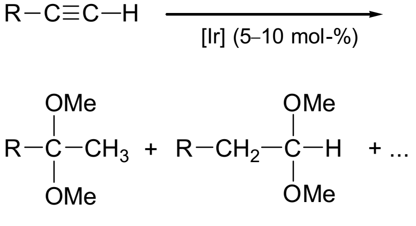
Iridium-catalyzed addition of methanol to terminal alkynes

The 18-crown-6 (18C6) ether adduct of sodium hexachloroiridate $[Na(18C6)]_2[IrCl_6]\cdot xH_2O$ (**1**) was found to catalyze an addition of methanol to a variety of nonfunctionalized alkynes RC≡CH (R = H, ^{n}Pr, ^{n}Bu, ^{n}Pen, Ph, $HC{\equiv}C(CH_2)_4$) yielding mainly the Markovnikov addition products (ketals) (>90%). In contrast, the regioselectivity in an addition to functionalized terminal alkynes RC(O)C≡CH (R = OMe, Me) was found to be towards *anti*-Markovnikov products (70–93%).



$$R{-}C{\equiv}C{-}H \xrightarrow[\text{[Ir] (5–10 mol-\%)}]{\text{MeOH, 40–60 °C}} R{-}\underset{\text{OMe}}{\overset{\text{OMe}}{C}}{-}CH_3 + R{-}CH_2{-}\underset{\text{OMe}}{\overset{\text{OMe}}{C}}{-}H + \ldots$$

Hangning Chen, Rong Li, Huanling Wang, Jiawei Liu, Fushan Wang, Jiantai Ma

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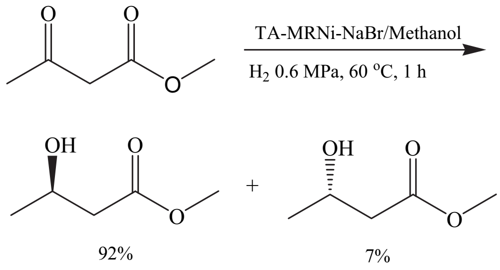
Highly efficient enantio-selective hydrogenation of methyl acetoacetate over chirally modified Raney nickel catalytic system

Using methanol containing an appropriate amount of NaBr as the reaction medium, a high optical yield of 85% was achieved in the enantio-selective hydrogenation of methyl acetoacetate over a tartaric acid modified Raney nickel catalyst under comparatively mild conditions (0.6 MPa, 60 °C, 1 h). The characterization data indicated that the improved TA-MRNi-NaBr catalyst had a lower weight ratio of Al–Ni, higher total surface area and more acid-corrosion on its surface.



G. Blanco-Brieva, M.C. Capel-Sanchez, J.M. Campos-Martin, J.L.G. Fierro

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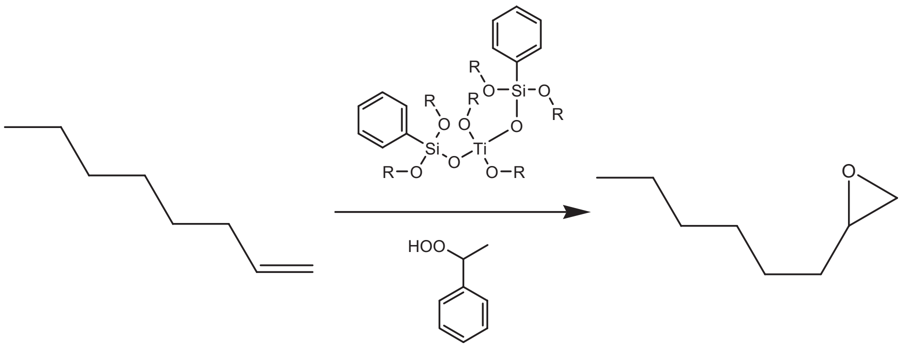
Effect of precursor nature on the behavior of titanium-polysiloxane homogeneous catalysts in primary alkene epoxidation



Bogusława Łęska, Radosław Pankiewicz, Grzegorz Schroeder, Angelamaria Maia

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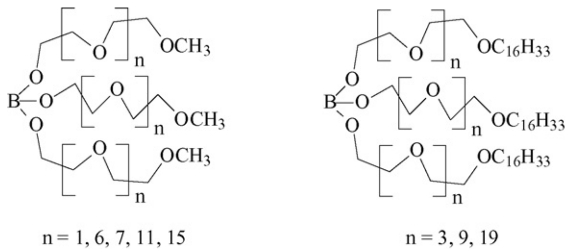
Application of a new class B-podands in solid–liquid phase transfer catalysis

We have reported the systematic study on the use of boron polypodands (B-podands) as catalyst in a series of anion promoted reactions (nucleophilic substitution, reduction, *N*- and *O*-alkylation) in chlorobenzene, toluene and acetonitrile solutions carried out under solid–liquid (SL) phase transfer catalysis (PTC) conditions.



Tong Dong-ge, Chu Wei, Luo Yong-yue, Chen Hong, Ji Xiao-yang

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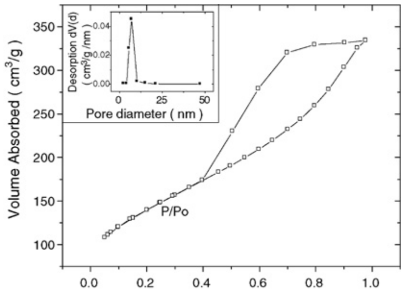
Preparation and characterization of amorphous Co-B catalysts with mesoporous structure

Novel mesoporous Co-B alloy catalyst was prepared. The catalyst exhibited higher cinnamaldehyde conversion and cinnamyl alcohol selectivity than the regular Co-B, which is attributed to its larger specific surface area and stronger affinity to C=O. Furthermore, it showed good cycle performance due to its preserved mesoporous structure during cycling.



Chen Chen, Ying-Feng Li, Lian-Ming Yang

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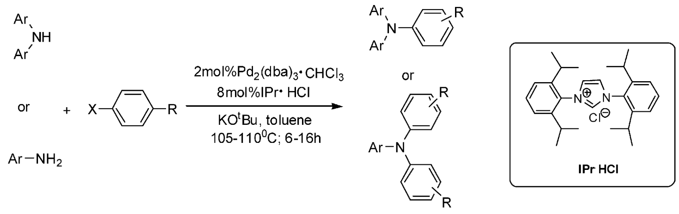
Efficient synthesis of triarylamines catalyzed by palladium/*N*-heterocyclic carbene

A palladium(0)/imidazolium salt system as catalyst precursor proved to be effective, under the appropriately selected reaction conditions, for *N*-arylation of diarylamines and anilines with unactivated aryl bromides or chlorides to afford triarylamine derivatives. In most cases, excellent yields were achieved.



Masaaki Nabika, Seiki Kiuchi, Tatsuya Miyatake, Ken-Ichi Okamoto, Kiyoshi Fujisawa

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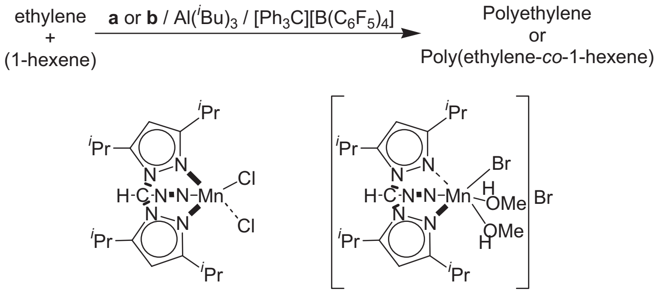
Manganese(II) halogeno complexes with neutral tris(3,5-diisopropyl-1-pyrazolyl)methane ligand: Synthesis and ethylene polymerization



a: $[Mn(Cl_2)(L1')]$ b: $[Mn(Br)(L1')(MeOH)_2](Br)$

Xiao-Yuan Liao, Dong-Bo Cao, Sheng-Guang Wang, Zhong-Yun Ma, Yong-Wang Li, Jianguo Wang, Haijun Jiao

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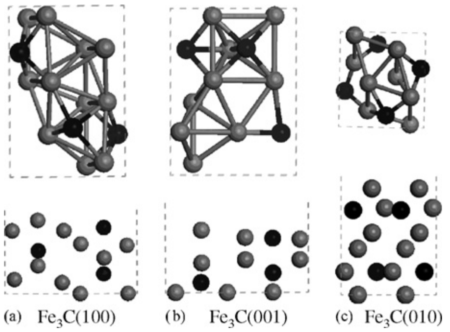
Density functional theory study of CO adsorption on the (1 0 0), (0 0 1) and (0 1 0) surfaces of Fe_3C



(a) $Fe_3C(100)$ (b) $Fe_3C(001)$ (c) $Fe_3C(010)$

Zhi-Ce Chen, Xin-Ping Hui, Chao Yin, Lu-Ning Huang, Peng-Fei Xu, Xiao-Xia Yu, Shao-Yi Cheng

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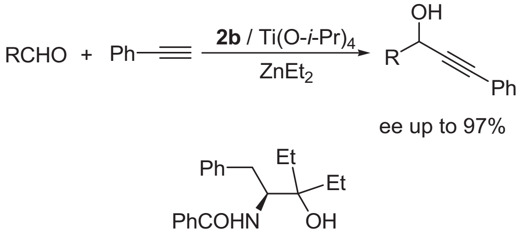
Highly enantioselective addition of phenylacetylene to aldehydes catalyzed by titanium(IV) complexes of β-hydroxy amides

A series of chiral β-hydroxy amide ligands were synthesized from L-amino acids by facile approaches. The enantioselective addition of phenylacetylene to aldehydes catalyzed by titanium(IV) complexes of these new chiral ligands were investigated. Excellent enantioselectivities were obtained for the desired propargyl alcohols with enantiomeric excesses values up to 97%.



2b

Lin Wu, Aimin Li, Guandao Gao, Zhenghao Fei, Shirong Xu, Quanxing Zhang

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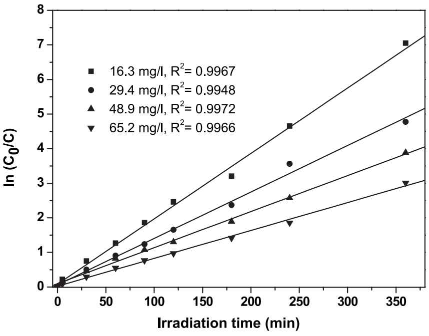
Efficient photodegradation of 2,4-dichlorophenol in aqueous solution catalyzed by polydivinylbenzene-supported zinc phthalocyanine

Photodegradation of 2,4-dichlorophenol in aerated aqueous solution catalyzed by polydivinylbenzene-supported zinc phthalocyanine has been investigated. The reaction followed pseudo-first-order kinetics. The heterogeneous photodegradation proceeded through formation of more biodegradable low molecular weight compounds. Hydroxyl radical and superoxide anion radical other than singlet oxygen were probably generated during the photodegradation of 2,4-dichlorophenol.



Rafael Luque, Juan Manuel Campelo, Diego Luna, Jose Maria Marinas, Antonio Angel Romero

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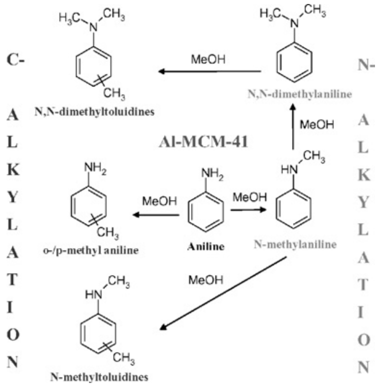
Catalytic performance of Al-MCM-41 materials in the *N*-alkylation of aniline



Sachindranath Pal, Wen-Shu Hwang, Ivan J.B. Lin, Chen-Shiang Lee

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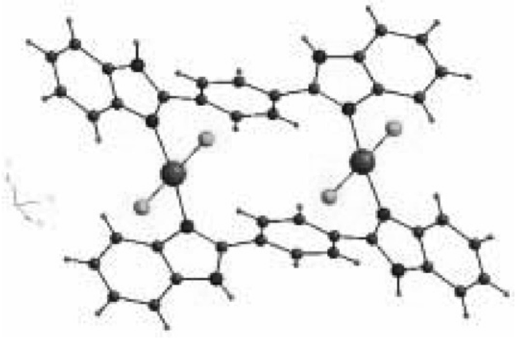
Benzene benzimidazole containing Pd(II) metallacycle: Synthesis, X-ray crystallographic characterization and its use as an efficient Suzuki coupling catalyst

A first example of a highly stable benzimidazole N-donor dinuclear palladacycle complex is reported. The complex catalyzed biaryl formation reaction effectively in MeOH at room temperature.



Belén Blanco, Marcial Moreno-Mañas, Roser Pleixats, Ahmad Mehdi, Catherine Reyé

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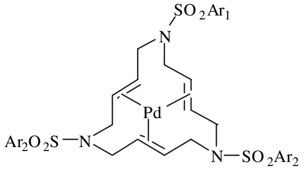
Organic–inorganic hybrid materials containing 15-membered azamacrocyclic triolefinic palladium(0) complexes. Preparation and activity as recoverable catalysts in Suzuki cross-couplings

Several hybrid organic–inorganic materials containing macrocyclic triolefinic palladium(0) complexes are prepared by sol–gel processes. They are active and reusable catalysts in Suzuki cross-coupling reactions.



$Ar_1 = p\text{-}C_6H_4\text{-NH-spacer-}SiO_{1.5} \cdot n\,SiO_2$

Ar_2 = 2,4,6-triisopropylphenyl

Mihir K. Chaudhuri, Sahid Hussain

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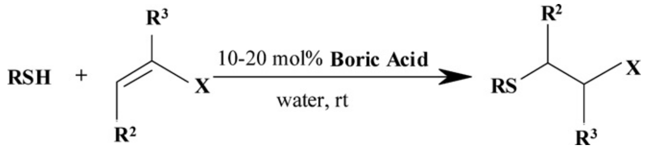
Boric acid catalyzed thia-Michael reactions in water or alcohols

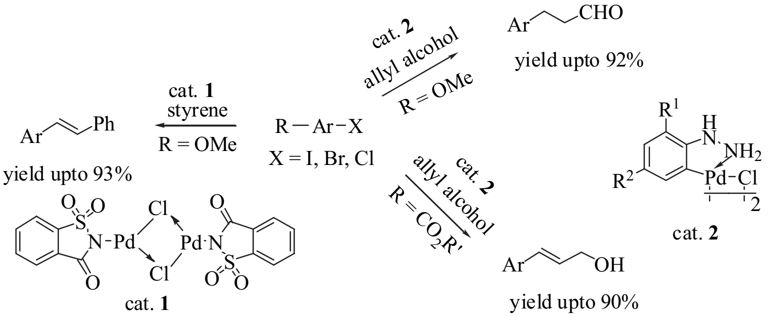


N.S.C. Ramesh Kumar, I. Victor Paul Raj, A. Sudalai

Journal of Molecular Catalysis A: Chemical 269 (2007) 218

Sulfonamide- and hydrazine-based palladium catalysts: Stable and efficient catalysts for C–C coupling reactions in aqueous medium

A novel family of sulfonamide-based palladium complexes and phenylhydrazine-based palladacycles from inexpensive and readily available ligands has been synthesized. These Pd catalysts were used for C–C bond forming reactions such as Suzuki, Heck, Sonogashira reactions and arylation of allyl alcohols in the aqueous medium.



N.S. Linge Gowda, M.N. Kumara, D. Channe Gowda, Kanchugara Koppal S. Rangappa, Netkal M. Made Gowda

Journal of Molecular Catalysis A: Chemical 269 (2007) 225

N-Bromosuccinimide assisted oxidation of hydrophobic tetrapeptide sequences of elastin: A mechanistic study

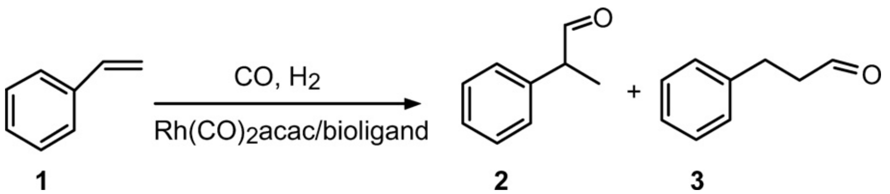
The repeating sequences of elastin, glycyl–glycyl–alanyl–proline (GGAP), glycyl–glycyl–isoleucyl–proline (GGIP) and more hydrophobic glycyl–glycyl–phenylalanyl–proline (GGPP), were synthesized by classical solution phase methods and characterized. The kinetics of oxidation of tetrapeptides (TPs) and their constituent amino acids (AAs) by *N*-bromosuccinimide (NBS) was studied in the presence of perchlorate ions in acidic medium at 28 °C. The reaction was followed spectrophotometrically at λ_{max} = 240 nm. The reactions follow identical kinetics, being first order each in [NBS], [AA] and [TP]. No effect on the rate of [H$^+$], reduction product [succinimide] and ionic strength was observed. Effects of dielectric constant of the medium and the added anions such as chloride and perchlorate were studied. Activation parameters have been computed. The oxidation products of the reaction were isolated and characterized. The proposed mechanism is consistent with the experimental results. An apparent correlation was noted between the rate of oxidation and the hydrophobicity of AAs and TPs.

S. Paganelli, M. Marchetti, M. Bianchin, C. Bertucci

Journal of Molecular Catalysis A: Chemical 269 (2007) 234

Aqueous biphasic hydroformylation catalyzed by rhodium carbonyl complexes modified with bioligands

Some amino acids and oligopeptides have been used as ligands for Rh(CO)$_2$(acac) in the aqueous biphasic hydroformylation of styrene. The water soluble catalytic systems obtained by using bioligands containing an SH moiety, as L-cysteine and the oligopeptide glutathione, in its reduced form, showed a good activity that remained practically unchanged during three recycled experiments.

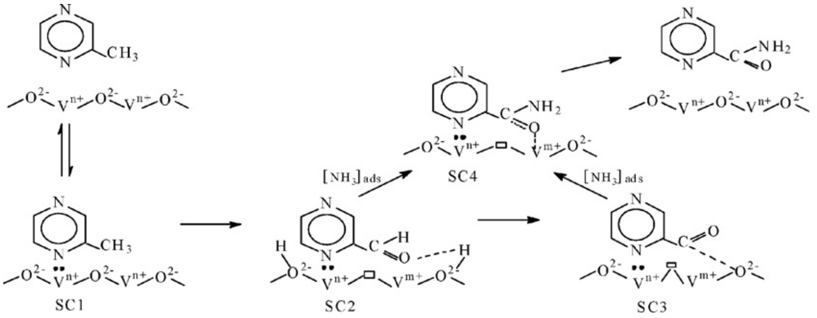


V.M. Bondareva, T.V. Andrushkevich, E.A. Paukshtis, N.A. Paukshtis, A.A. Budneva, V.N. Parmon

Journal of Molecular Catalysis A: Chemical 269 (2007) 240

Investigation of the reaction mechanism of methylpyrazine ammoxidation on vanadia–titania catalyst by FTIR *in situ*

The mechanism of methylpyrazine ammoxidation on a vanadia–titania catalyst has been studied by *in situ* FTIR spectroscopy. The structure of surface intermediates has been identified and the sequence of their transformation in the temperature range of 150–230 °C has been ascertained.

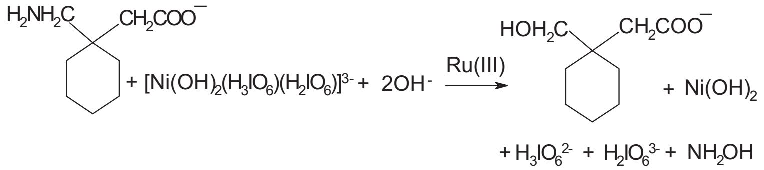


Chanabasayya V. Hiremath, Deepak C. Hiremath, Sharanappa T. Nandibewoor

Journal of Molecular Catalysis A: Chemical 269 (2007) 246

Ruthenium(III) catalysed oxidation of gabapentin (neurontin) by diperiodatonickelate(IV) in aqueous alkaline medium: A kinetic and mechanistic study

The kinetics of Ru(III) catalysed oxidation of neuroleptic drug, gabapentin by diperiodatonickelate(IV) (DPN) in alkaline medium at 298 K. The oxidation reaction in alkaline medium has been shown to proceed via a Ru(III)–gabapentin complex, which further reacts with deprotonated form of DPN in a rate determining step, which is followed by other fast steps to give the products. The oxidation products are 1-(hydroxymethyl) cyclohexane acetic acid and Ni(II) which are identified by IR and NMR studies.

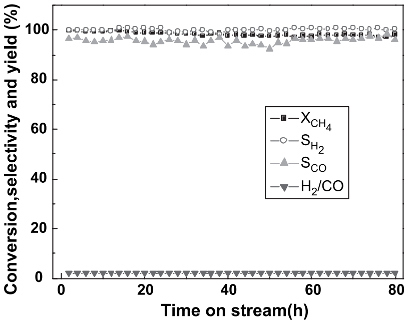


Cuili Guo, Xiaoling Zhang, Jinli Zhang, Yiping Wang

Journal of Molecular Catalysis A: Chemical 269 (2007) 254

Preparation of La_2NiO_4 catalyst and catalytic performance for partial oxidation of methane

Performances of La_2NiO_4 perovskite, prepared using citric acid complex method, as catalysts for partial oxidation of methane to synthesis gas have been studied. The catalysts were characterized by BET, XRD, TG/DTG and SEM. Among catalysts tested, the catalyst La_2NiO_4 calcinated at 850 °C with the molar ratio of La:Ni:CA = 2:1:3 exhibits the best activity and excellent stability as well as very low coke formation.



Stability testing of La_2NiO_4 catalyst for POM Reaction conditions: 800°C,$CH_4/O_2/N_2$= 2/1/4, flow rate of 98ml/min