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Contents lists available at ScienceDirect

Journal of Molecular Catalysis A: Chemical

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Articles

Takeo Yamamoto, Chie Shikada, Shojiro Kaita, Tardif Olivier, Yoochiroh Maruyama, Yasuo Wakatsuki

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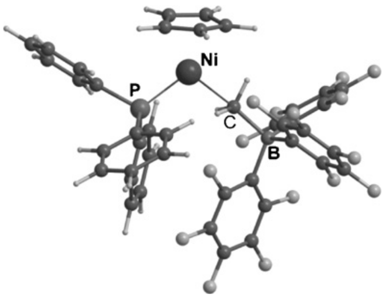
Role of $B(C_6F_5)_3$ in activating the nickel-methyl complex $(\eta^5\text{-}C_5H_5)Ni(CH_3)(PPh_3)$ to initiate the vinyl polymerization of norbornene

The Lewis acid $B(C_6F_5)_3$ attacks $(\eta^5\text{-}C_5H_5)Ni(CH_3)(PPh_3)$ at the Ni-bound methyl group to form a contact ion-pair complex with Ni-(μ-CH_3)-B bond. Successive pathways to generate an active species that can initiate the vinyl polymerization of norbornene are presented based on the reactions of the ion-pair complex.



A. Drelinkiewicz, W. Stanuch, A. Knapik, A. Ghanem, R. Kosydar, A. Bukowska, W. Bukowski

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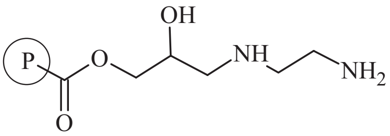
Amine groups functionalized gel-type resin supported Pd catalysts: Physicochemical and catalytic properties in hydrogenation of alkynes

Amine groups—functionalized gel-type resin (FCN) supported Pd catalysts exhibit attractive performance in hydrogenation of alkynes reagents, 2-butyne-1,4-diol and phenylacetylene. The selectivity to desired alkenes products attained ca. 94% at almost complete conversion of alkynes. This performance is unchanged under the recycling use of catalysts.



Mônica C.G. Albuquerque, Diana C.S. Azevedo, Célio L. Cavalcante Jr., José Santamaría-González, Josefa M. Mérida-Robles, Ramón Moreno-Tost, Enrique Rodríguez-Castellón, Antonio Jiménez-López, Pedro Maireles-Torres

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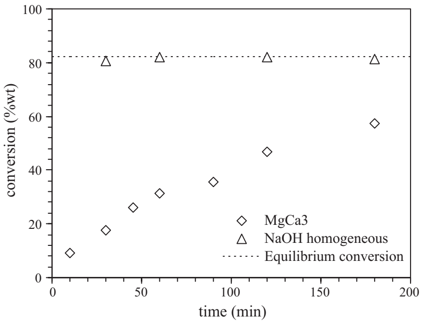
Transesterification of ethyl butyrate with methanol using MgO/CaO catalysts

A series of mixtures of MgO/CaO was prepared and characterized. The heterogeneous transesterification of ethyl butyrate with methanol, as a model reaction for biodiesel production, was performed, reaching conversions as high as 60%. Moreover, unlike commercial CaO, no lixiviation of the active phase was detected.



doi:10.1016/S1381-1169(09)00049-1

Wenjin Xu, Hao Guo, Jun Zhang, Qifeng Zhu, Xianming Hu

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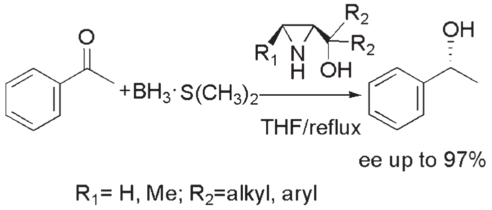
Asymmetric reduction of acetophenone using α,α-disubstituted aziridinemethanols and borane

Enantioselective reduction of acetophenone using α,α-disubstituted aziridinemethanols as catalysts proceeded with high ee values under more facile reaction conditions. Aziridinemethanols α,α-disubstituted with electron-withdrawing groups displayed much higher enantioselectivity than those α,α-disubstituted with electron-donating groups under the same conditions of solvent, temperature and the amount of catalyst, which allowed the rational modification of catalyst structure to achieve optimal enantioselectivity.



Dipak Kumar Dutta, Pratap Chutia, Bhaskar J. Sarmah, Bibek J. Borah, Biswajit Deb, J. Derek Woollins

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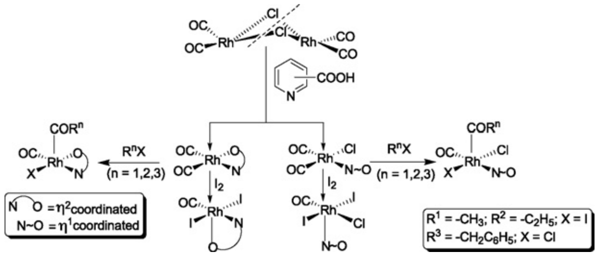
Rhodium carbonyl complexes containing pyridine carboxylic acid ligands: Reactivity towards various electrophiles and catalytic activity

[Rh(CO)$_2$Cl]$_2$ reacts with pyridine carboxylic acid ligands to yield rhodium(I) dicarbonyl chelate complex [Rh(CO)$_2$(L$^{/}$)] {L$^{/}$ = η^2-(N,O) coordinated Py-2-COO$^-$} and non-chelate complexes [Rh(CO)$_2$ClL$^{//}$]{L$^{//}$ = η^1-(N) co-ordinated Py-COOH}. The complexes undergo oxidative addition (**OA**) with different electrophiles such as CH_3I, C_2H_5I, $C_6H_5CH_2Cl$ and I_2. The complexes show higher efficiency as catalyst for carbonylation of methanol compared to the industrially used species [Rh(CO)$_2$I$_2$]$^-$.



Xiao-zhi Liu, Shi-wei Lu

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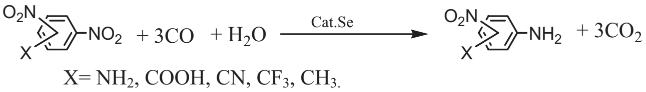
Selective formation of nitroanilines by selenium-catalyzed monoreduction of dinitrobenzenes with CO/H_2O

Nitroanilines are synthesized via selenium-catalyzed monoreduction of dinitrobenzenes with CO/H_2O. These reactions can proceed with high yield of desired nitroanilines not only under high pressure but also under atmospheric pressure.



Jing Guan, Gang Yang, Danhong Zhou, Weiping Zhang, Xianchun Liu, Xiuwen Han, Xinhe Bao

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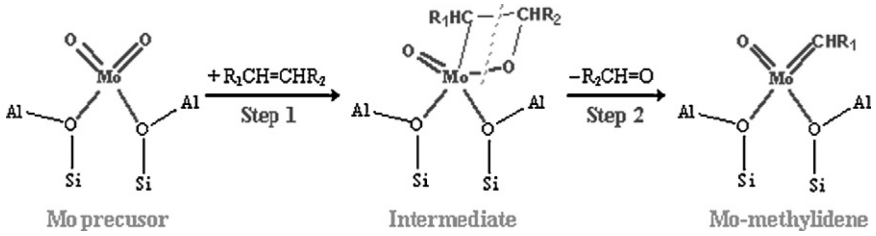
The formation mechanism of Mo-methylidene species over Mo/HBeta catalysts for heterogeneous olefin metathesis: A density functional theory study

Density functional calculations were employed to determine the formation mechanisms of the Mo-methylidene species in Mo/HBeta zeolite catalysts. It was found that both free energy barriers and reaction heats for the whole processes were lower in the Mo(VI) rather than in the Mo(V) active site, indicating that the Mo(VI) active site is more efficient to produce the Mo(VI)-methylidene species over the Mo/HBeta catalysts. Furthermore, the reactivities of the Mo active sites with different oxidation states were elucidated by the electronic properties of the O$_b$-ligands bonded to the Mo centers.



P. Centomo, M. Zecca, M. Kralik, D. Gasparovicova, K. Jerabek, P. Canton, B. Corain

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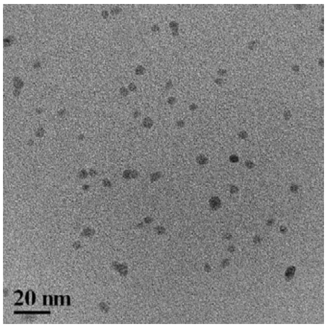
Cross-linked poly-vinyl polymers *versus* polyureas as designed supports for catalytically active M^0 nanoclusters. Part II. Pd^0/cross-linked poly-vinyl polymers *versus* Pd^0/EnCat™30NP in mild hydrogenation reactions

New resin based metal catalysts favourably compared with the commercially available Pd/EnCat™30NP catalyst.



Jinzhi Liu, Jun Ling, Xin Li, Zhiquan Shen

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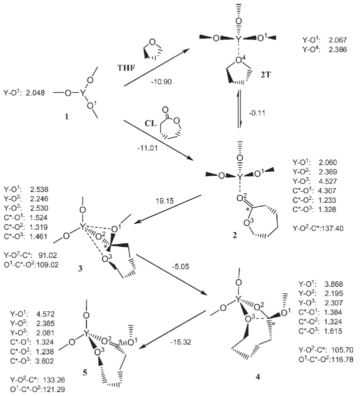
Monomer insertion mechanism of ring-opening polymerization of ε-caprolactone with yttrium alkoxide intermediate: A DFT study

A four-step coordination-insertion mechanism of ε-caprolactone (CL) insertion into a Y–OCH_3 bond was investigated. The coordination of CL onto yttrium center led to a nucleophilic addition, followed by an intramolecular alkoxide ligand exchange. A monomer insertion was completed by the CL ring opening via acyl–oxygen bond cleavage. The formation of the five-coordinated yttrium intermediate was the rate-determining step.



Ronald Vargas, Oswaldo Núñez

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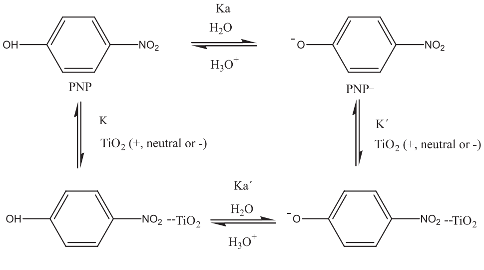
Hydrogen bond interactions at the TiO_2 surface: Their contribution to the pH dependent photo-catalytic degradation of *p*-nitrophenol

With adsorption equilibrium constants and the pK_a value of PNP in solution, thermodynamic cycles are established in order to obtain the pK_a of PNP when it is adsorbed on positively charged, neutral and negatively charged TiO_2 surfaces. From these pK_a values useful information on the PNP–TiO_2 interaction is readily obtained. The k_{obs} vs. pH profile predicts an efficient photo-catalytic PNP degradation at pH > 8.



$$pKa' = pKa + \log K - \log K'$$

Eunyoung Bae, Naoya Murakami, Teruhisa Ohno

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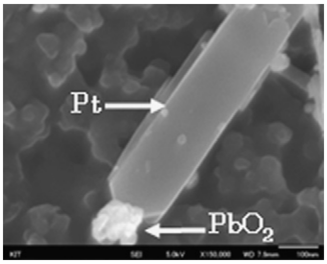
Exposed crystal surface-controlled TiO_2 nanorods having rutile phase from $TiCl_3$ under hydrothermal conditions

The surface chemistry of the rutile TiO_2 particles was also investigated. From photodeposition of Pt and PbO_2, we suggest that the (1 1 0) face provides reductive sites and that the (1 1 1) face provides oxidative sites. The results suggested that the crystal faces improve the separation of electrons and holes, resulting in improvement of photocatalytic activity.



Ching-Tu Chang, Biing-Jye Liaw, Yu-Pei Chen, Yin-Zu Chen

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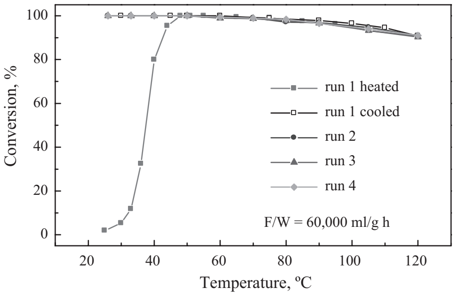
Characteristics of Au/Mg_xAlO hydrotalcite catalysts in CO selective oxidation

The 2%Au/Mg_2AlO hydrotalcite catalyst exhibited interesting behavior in the CO selective oxidation in excess hydrogen. The CO conversion increased with temperature up to complete conversion at around 48 °C, and the catalyst retained its high activity for complete conversion as the temperature decreased to room temperature and even during the repeated heating and cooling runs for 120 h.



Silvana T. Castaman, Shirley Nakagaki, Ronny R. Ribeiro, Kátia J. Ciuffi, Sueli M. Drechsel

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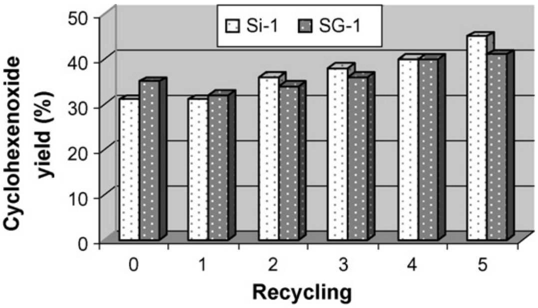
Homogeneous and heterogeneous olefin epoxidation catalyzed by a binuclear Mn(II)Mn(III) complex

The catalytic performance of the binuclear manganese complex Mn(II)Mn(III) in epoxidation reactions was evaluated for both homogeneous and heterogeneous systems. The obtained results reveals good performance of the complex as epoxidation catalyst for the substrates cyclohexene (26–39%) and cyclooctene (29–74%). The solids with the immobilized complex have shown good reutilization capacity.



ChaoFen Yang, HeYan Jiang, Jian Feng, HaiYan Fu, RuiXiang Li, Hua Chen, XianJun Li

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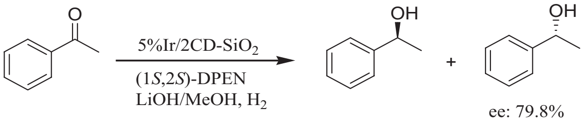
Asymmetric hydrogenation of acetophenone catalyzed by cinchonidine stabilized Ir/SiO_2

A series of silica (SiO_2) supported iridium catalysts stabilized by cinchona alkaloids was prepared and firstly applied in the heterogeneous asymmetric hydrogenation of acetophenone. In the presence of (1*S*,2*S*)-diphenylethylenediamine ((1*S*,2*S*)-DPEN)) as chiral modifier, the cinchonidine (CD) stabilized catalyst 5%Ir/2CD-SiO_2 exhibits excellent catalytic performance, the ee value of (*R*)-phenylethanol achieving 79.8%.



I. Atribak, A. Bueno-López, A. García-García

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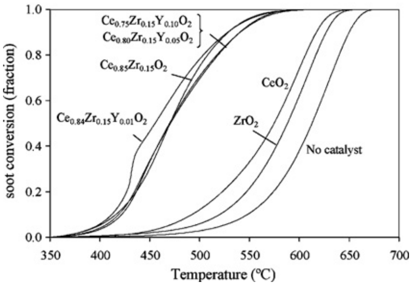
Role of yttrium loading in the physico-chemical properties and soot combustion activity of ceria and ceria–zirconia catalysts

$Ce_{1-x}Y_xO_2$ and $Ce_{0.85-x}Zr_{0.15}Y_xO_2$ mixed oxides have been prepared, characterised and tested for catalysed soot oxidation. $Ce_{0.84}Zr_{0.15}Y_{0.01}O_2$ is the most active catalyst, and higher yttrium loading ($x = 0.05–0.12$) is less effective than $x = 0.01$ because yttrium is mainly accumulated at the surface of the particles and hinders the catalytic activity of cerium.



Linda Aschwanden, Tamas Mallat,
Jan-Dierk Grunwaldt, Frank Krumeich,
Alfons Baiker

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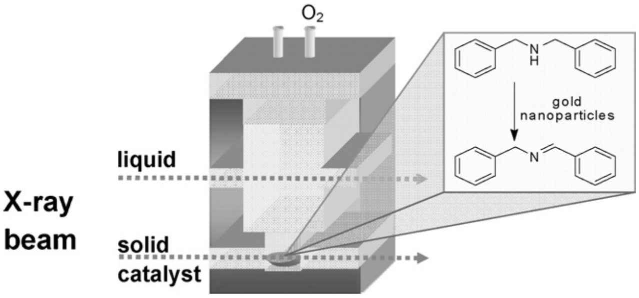
Gold-catalyzed aerobic oxidation of dibenzylamine: Homogeneous or heterogeneous catalysis?

Gold nanoparticles formed in situ from Au(OAc)$_3$ show excellent activity in the oxidation of dibenzylamine to imine with dioxygen. Evolution of the active gold species is followed by in situ XANES and confirmed by electron microscopy.



Li Yan, Yun J. Ding, Li W. Lin, He J. Zhu,
Hong M. Yin, Xian M. Li, Yuan Lu

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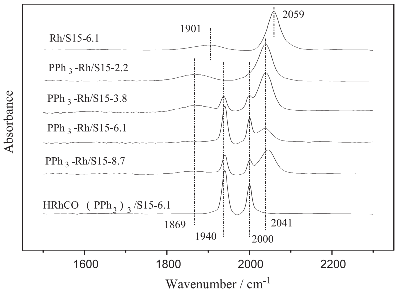
In situ formation of HRh(CO)$_2$(PPh$_3$)$_2$ active species on the surface of a SBA-15 supported heterogeneous catalyst and the effect of support pore size on the hydroformylation of propene

A method of in situ formation of HRh(CO)$_2$(PPh$_3$)$_2$ active species on the surface of heterogeneous catalyst has been developed and confirmed. The amount of active species can be controlled by the support pore size. The PPh$_3$-Rh/SBA-15 catalyst has been employed in propylene hydroformylation to be highly active, selective, stable, easily workable and recyclable.



Angel B. Rivas, Jesús J. Pérez-Torrente,
Alvaro J. Pardey, Anna M. Masdeu-Bultó,
Montserrat Diéguez, Luis A. Oro

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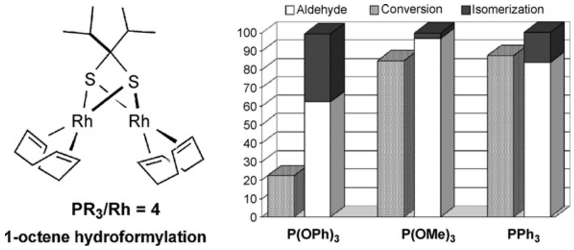
Hydroformylation of oct-1-ene catalyzed by dinuclear *gem*-dithiolato-bridged rhodium(I) complexes and phosphorus donor ligands

A series of dinuclear compounds [Rh$_2$(μ-S$_2$CR$_1$R$_2$)(cod)$_2$] having bridging *gem*-dithiolato ligands (R^1, R^2–(CH$_2$)$_4$–, –(CH$_2$)$_5$–; R^{1}R^{2}Bn, ^{i}Pr) in the presence of monodentate phosphine or phosphite ligands are efficient catalyst precursors for the hydroformylation of oct-1-ene under mild conditions. The catalytic activity is strongly influenced both by the structure of catalyst precursor and the P/Rh ratio being the precursors containing acyclic *gem*-dithiolato ligands considerably more active. Spectroscopic studies under pressure showed that mononuclear species formed under catalytic conditions are most likely responsible for the observed catalytic activity.



Rocío Redón, N.G. García-Peña,
V.M. Ugalde-Saldivar, J.J. García

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Palladium-triazine aminoalcohol nanocomposite, its reactivity on Heck reaction

The composite Pd-G0THT shows a high yield of *trans*- and *cis*-stilbene products activating even chlorobenzene in Heck reaction, mainly attributed to nanoparticle size reached inside the dendrimer.