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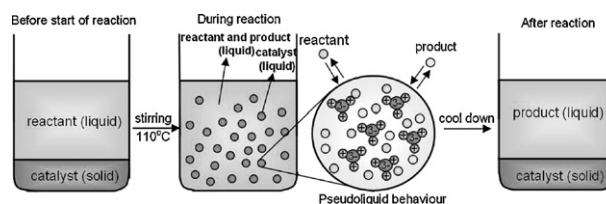
Articles

Yan Leng, Jun Wang, Dunru Zhu, Yajing Wu, Pingping Zhao

Journal of Molecular Catalysis A: Chemical 313 (2009) 1

Sulfonated organic heteropolyacid salts: Recyclable green solid catalysts for esterifications

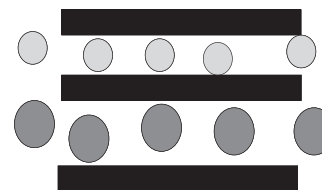
In the esterification of monocarboxylic acid with monohydric alcohol, propane sulfonate functionalized organic heteropolyacid (HPA) salts act as heterogeneous catalysts presenting high activity, easy recover and well reuse. The green process is mostly due to the solid nature and pseudoliquid behaviour of HPA salts, making the functional acidic species in the bulk of salts to fully act as active centers for the reactions.



R. Roque-Malherbe, V. Ivanov

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Codiffusion and counterdiffusion of para-xylene and ortho-xylene in a zeolite with 10 MR/12 MR interconnected channels. An example of molecular traffic control

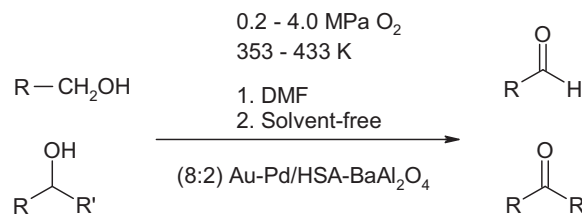


P.G.N. Mertens, S.L.F. Corthals, X. Ye, H. Poelman, P.A. Jacobs, B.F. Sels, I.F.J. Vankelecom, D.E. De Vos

Journal of Molecular Catalysis A: Chemical 313 (2009) 14

Selective alcohol oxidation to aldehydes and ketones over base-promoted gold–palladium clusters as recyclable quasihomogeneous and heterogeneous metal catalysts

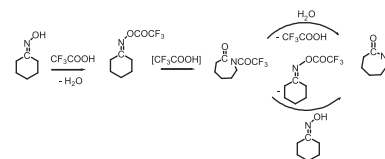
Bimetallic gold–palladium clusters, with an average size of 1.9 nm and composed of 80 mol% gold, proved to be active, selective and durable metal catalysts for the oxidation with O₂ of aliphatic, allylic and benzylic alcohols to the corresponding aldehydes and ketones, both as such as quasihomogeneous catalysts applied in DMF and as heterogeneous catalysts after immobilization on a basic high surface area BaAl₂O₄ spinel support for use in solvent-free conditions.



L. Ronchin, A. Vavasori*Journal of Molecular Catalysis A: Chemical* 313 (2009) 22

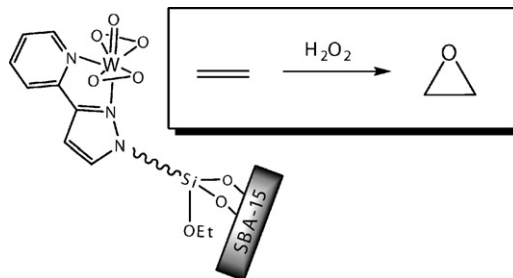
On the mechanism of the organocatalyzed Beckmann rearrangement of cyclohexanone oxime by trifluoroacetic acid in aprotic solvent

The Beckmann rearrangement of cyclohexanone oxime to ϵ -caprolactam catalyzed by trifluoroacetic acid in aprotic solvents is described. The identification of the key intermediate and its role in the catalysis is reported.

**Jianyuan Tang, Lei Wang, Gang Liu, Yan Liu, Yazhuo Hou, Wenxiang Zhang, Mingjun Jia, Werner R. Thiel***Journal of Molecular Catalysis A: Chemical* 313 (2009) 31

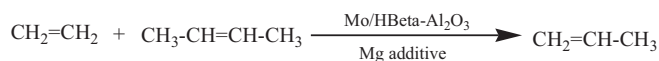
Mesoporous SBA-15 materials modified with oxodiperoxo tungsten complexes as efficient catalysts for the epoxidation of olefins with hydrogen peroxide

An oxodiperoxo tungsten complex modified SBA-15 material is active catalyst for the epoxidation of cyclooctene with H_2O_2 as the oxidant, and it exhibits relatively high stability against leaching of active tungsten species. Moreover, this catalyst showed very high efficiency for H_2O_2 utilization, and its catalytic activity could be further improved by using solvent mixtures of CH_3CN and CH_3COOH .

**Xiujie Li, Weiping Zhang, Shenglin Liu, Sujuan Xie, Xiangxue Zhu, Xinhe Bao, Longya Xu***Journal of Molecular Catalysis A: Chemical* 313 (2009) 38

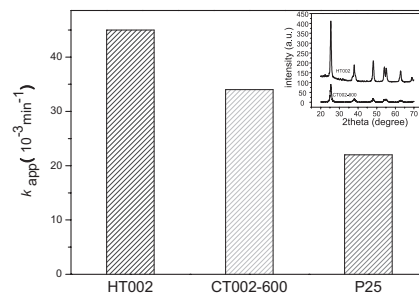
Promoting effect of Mg in supported Mo/HBeta- Al_2O_3 catalyst for cross-metathesis of ethene and butene-2 to propene

Addition of Mg to Mo/HBeta- Al_2O_3 olefin metathesis catalysts may change the acidity and surrounding symmetry of Mo species. Better catalyst stability could be obtained with the Mg content in the range of 1–2 wt% owing to the elimination of weak acid sites. High Mg loading increases the reducibility difficulty of Mo species which leads to poor performances of the catalyst in the metathesis reaction of ethene and butene-2 to propene.

**C. Jin, R.Y. Zheng, Y. Guo, J.L. Xie, Y.X. Zhu, Y.C. Xie***Journal of Molecular Catalysis A: Chemical* 313 (2009) 44

Hydrothermal synthesis and characterization of phosphorous-doped TiO_2 with high photocatalytic activity for methylene blue degradation

Phosphorous-doped titania was synthesized by a one step hydrothermal method. These samples exhibit much higher crystallinity compared to those prepared by conventional calcination method. The best performance for methylene blue degradation was obtained on HT002 (2% P:Ti atomic ratio), which is 30% higher than that of the sample calcined at 600 °C (CT002-600) and twice that of P25.

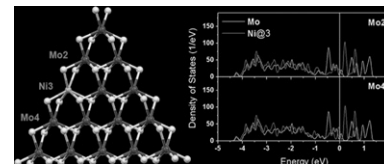


**Carolina Zuriaga-Monroy,
José-Manuel Martínez-Magadán, Estrella Ramos,
Rodolfo Gómez-Balderas**

Journal of Molecular Catalysis A: Chemical 313 (2009) 49

A DFT study of the electronic structure of cobalt and nickel mono-substituted MoS₂ triangular nanosized clusters

Ni promotional effect is observed as an increase of projected density of states above the Fermi level, favoring the donation step in the C–S breaking bond of molecules under HDS process. The projected density of states below the Fermi level is diminished, reducing the states available for charge back-donation.

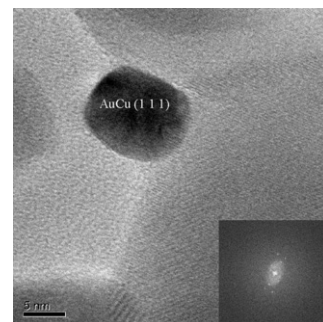


**Feg-Wen Chang, Ti-Cheng Ou, L. Selva Roselin,
Wun-Syong Chen, Szu-Chia Lai, Hsiao-Min Wu**

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Production of hydrogen by partial oxidation of methanol over bimetallic Au–Cu/TiO₂–Fe₂O₃ catalysts

Partial oxidation of methanol to produce H₂ was investigated over Au–Cu/TiO₂ and Au–Cu/TiO₂–Fe₂O₃ catalysts. The Au–Cu/TiO₂–Fe₂O₃ catalyst with Ti/Fe = 9/1 atomic ratio is more active compared to the Au–Cu/TiO₂ catalyst. The higher activity of Fe-containing catalyst was attributed to the stabilization of active gold species (Au^{δ+}) in the catalyst.

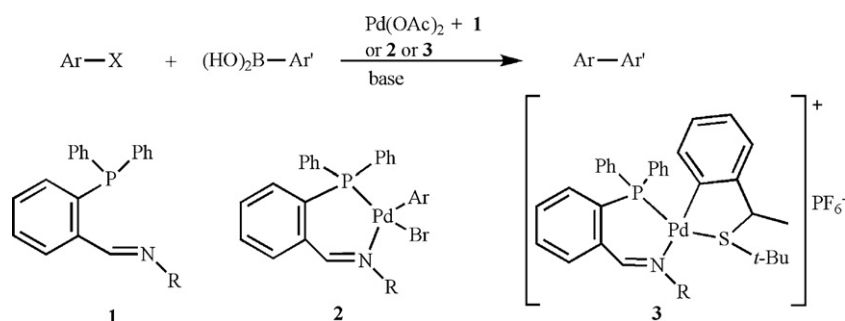


Sabrina M. Nobre, Adriano L. Monteiro

Journal of Molecular Catalysis A: Chemical 313 (2009) 65

Pd complexes of iminophosphine ligands: A homogeneous molecular catalyst for Suzuki–Miyaura cross-coupling reactions under mild conditions

Catalytic activity: **2** > Pd(OAc)₂ + **1** > **3**. Poisoning tests demonstrated that homogeneous mononuclear palladium species containing the iminophosphine ligand were responsible for the catalytic activity at 50 °C.

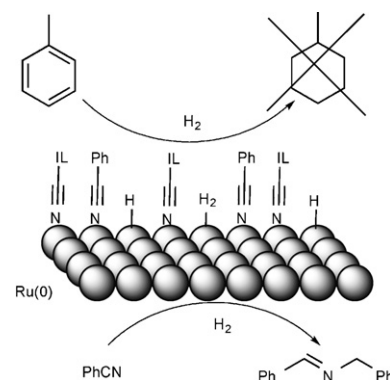


**Martin H.G. Precht, Jackson D. Scholten,
Jairton Dupont**

Journal of Molecular Catalysis A: Chemical 313 (2009) 74

Tuning the selectivity of ruthenium nanoscale catalysts with functionalised ionic liquids: Hydrogenation of nitriles

Nitrile groups are exclusively hydrogenated in the presence of ruthenium nanoparticles (2.2 ± 0.5 nm) prepared in nitrile-functionalised ionic liquids. On opposition, ruthenium nanoparticles in non-functionalised imidazolium ionic liquids promote preferentially the hydrogenation of the aromatic rings. The substrates bearing a nitrile group coordinated preferentially to the metal surface via the nitrile group rather than the arene moiety.

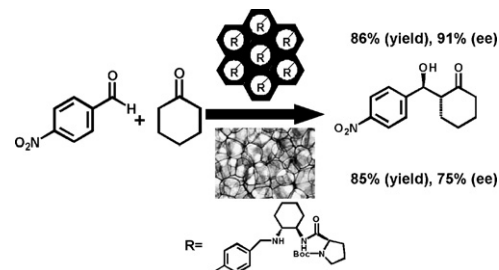


Jinsuo Gao, Jian Liu, Dongmei Jiang, Bing Xiao, Qihua Yang

Journal of Molecular Catalysis A: Chemical 313 (2009) 79

L-Prolinamide functionalized mesoporous silicas: Synthesis and catalytic performance in direct aldol reaction

The highly ordered 2D hexagonal mesostructure and disordered foam-like mesostructure mesoporous materials functionalized with L-prolinamide were obtained by using different silicon precursors in HAc–NaAc buffer solution. In asymmetric Aldol reaction of cyclohexanone and 4-nitrobenzaldehyde, the materials with ordered mesostructure exhibited higher enantioselectivity (91% ee) than that with disordered foam-like mesostructure (75% ee).

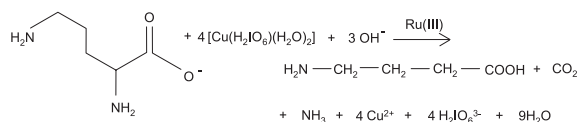


Jyothi C. Abbar, Shweta J. Malode, Sharanappa T. Nandibewoor

Journal of Molecular Catalysis A: Chemical 313 (2009) 88

Mechanistic aspects of uncatalyzed and ruthenium(III) catalyzed oxidation of DL-ornithine by copper(III) periodate complex in aqueous alkaline medium: A comparative kinetic study

The oxidation of DL-ornithine (OMH) by diperioiodocuprate(III) (DPC) both in the absence and presence of ruthenium (III) catalyst in alkaline medium at a constant ionic strength was studied spectrophotometrically. The stoichiometry was the same in both cases, i.e., [OMH]/[DPC] = 1:4. Suitable mechanisms were proposed. The active species of DPC and Ru(III) were found to be $[\text{Cu}(\text{H}_2\text{IO}_6)(\text{H}_2\text{O})_2]$ and $[\text{Ru}(\text{H}_2\text{O})_5\text{OH}]^{2+}$ respectively.

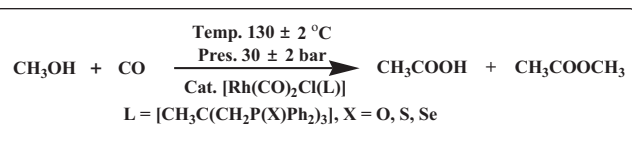


Dipak Kumar Dutta, J. Derek Woollins, Alexandra M.Z. Slawin, Amy L. Fuller, Biswajit Deb, Podma Pollov Sarmah, Madan Gopal Pathak, Dilip Konwar

Journal of Molecular Catalysis A: Chemical 313 (2009) 100

Rhodium(I) carbonyl complexes of chalcogen functionalized tripodal phosphines, $[\text{CH}_3\text{C}(\text{CH}_2\text{P}(\text{X})\text{Ph}_2)_3]$ {X = O, S, Se} and their reactivity

Three newly synthesized rhodium(I) carbonyl complexes of 1,1,1-tris(diphenylphosphinomethyl) ethanetrichalcogenide ligands undergo oxidative addition reactions with different electrophiles such as CH_3I , $\text{C}_2\text{H}_5\text{I}$ and $\text{C}_6\text{H}_5\text{CH}_2\text{Cl}$ to generate a mixture of isomeric Rh(III) complexes, and exhibit higher catalytic activity (TON = 1564–1723) in carbonylation of methanol compared to well-known Monsanto's species $[\text{Rh}(\text{CO})_2\text{I}]^-$ (TON = 1000).



Minghua Zhou, Jiaguo Yu, Huogen Yu

Journal of Molecular Catalysis A: Chemical 313 (2009) 107

Effects of urea on the microstructure and photocatalytic activity of bimodal mesoporous titania microspheres

Bimodal mesoporous TiO_2 microspheres with high photocatalytic activity for decomposition of acetone in air are prepared by a hydrothermal method and all prepared samples show bimodal pore-size distributions in the mesoporous region: smaller intra-aggregated pores with peak pore diameter of ca. 2 nm and larger inter-aggregated pores with peak pore diameter of ca. 12.5 nm.

