



Journal of Molecular Catalysis A: Chemical

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Jacques Muzart

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 Pd^{0-} and $Pd^{u}\text{-}catalyzed$ oxaheterocyclization of substrates having both an allylic leaving group and a hydroxylated tether

A review on the palladium-catalyzed intramolecular reactions leading to oxygenated heterocycles, from substrates having both an allylic leaving group and a hydroxylated tether is presented.



Marek Cypryk, Piotr Pospiech, Krzysztof Strzelec, Karolina Wasikowska, Janusz W. Sobczak

Soluble polysiloxanes of various architectures having various ligands have been used as supports for palladium catalysts. Their catalytic activity was tested in model Heck reactions.

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Soluble polysiloxane-supported palladium catalysts for the Mizoroki–Heck reaction





Sergey V. Sirotin, Alexander Yu. Tolbin, Irina F. Moskovskaya, Sergey S. Abramchuk, Larisa G. Tomilova, Boris V. Romanovsky

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Heterogenized Fe(III) phthalocyanine: Synthesis, characterization and application in liquid-phase oxidation of phenol





Renyang Zheng, Ying Guo, Chen Jin, Jinglin Xie, Yuexiang Zhu, Youchang Xie

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Novel thermally stable phosphorus-doped TiO₂ photocatalyst synthesized by hydrolysis of TiCl₄

A simple, low-cost and reproducible method was developed for the synthesis of novel thermally stable P-doped TiO_2 by liquid hydrolysis of $TiCl_4$ and ammonia, with hypophosphorous acid as the precursor of the dopant. Photocatalytic tests showed that the P-doped TiO_2 kept its superior specific activity at high calcination temperature (700–900 °C).



Benjaram M. Reddy, Gunugunuri K. Reddy, Lakshmi Katta

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Structural characterization and dehydration activity of CeO_2 -SiO₂ and CeO_2 -ZrO₂ mixed oxides prepared by a rapid microwave-assisted combustion synthesis method

 CeO_2 -SiO₂ and CeO_2 -ZrO₂ mixed oxides synthesized by a rapid microwave-assisted solution combustion synthesis method were characterized and evaluated for vapor phase dehydration of 4-methylpentan-2-ol at normal atmospheric pressure. Both catalysts exhibited interesting catalytic properties for this reaction.

Ag. Stamatis, D. Giasafaki, K.C. Christoforidis, Y. Deligiannakis, M. Louloudi

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The catalytic function of SiO₂-immobilized Mn(II)complexes for alkene epoxidation with H₂O₂ Manganese heterogeneous catalysts with symmetrical acetylacetone-based Schiff bases have been prepared by grafting and sol–gel procedure. They have been evaluated for alkene epoxidation with H_2O_2 showing remarkable effectiveness and selectivity towards epoxide formation in the presence of ammonium acetate. The developed heterogeneous catalysts preserve the coordination and catalytic properties of the active-homogeneous manganese catalysts for alkene epoxidation *vs.* the competitive H_2O_2 dismutation.



Bibek Jyoti Borah, Biswajit Deb, Podma Pollov Sarmah, Dipak Kumar Dutta

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Dicarbonylrhodium(I) complexes of benzoylpyridine ligands: Synthesis, reactivity and catalytic carbonylation reaction The three new Rh(I) carbonyl complexes of the type [Rh(CO)₂ClL]; L = 2-Benzoylpyridine, 3-Benzoylpyridine and 4-Benzoylpyridine have been synthesized, which undergo oxidative addition (**OA**) with different electrophiles such as CH₃I, C₂H₅I, and C₆H₅CH₂Cl. These complexes show higher catalytic activity (**TON** = 1529–1748) in carbonylation of methanol than well known Monsanto's species [Rh(CO)₂I₂]⁻ (**TON** = 1000).

| CH ₂ OH + CO | Temp. $130 \pm 2^{\circ}C$ Pres. 30 ± 2 bar, 1h CH ₄ COOH + CH ₂ COOCH ₄ |
|-------------------------|---|
| | Cat. [Rh(CO) ₂ Cl(L)] $I = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}$ |
| | |





Takayuki Komatsu, Kazunori Sou, Ken-ichi Ozawa

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Preparation and catalytic properties of fine particles of Pt-Ge intermetallic compound formed inside the mesopores of MCM-41 Fine particles of an intermetallic compound, PtGe, were created inside the mesopores of MCM-41. Their particle size had very narrow distribution around 1.5 nm. The comparable catalytic activity of PtGe/MCM-41 to that of Pt/MCM-41 indicates the nano-size effect in H_2 – D_2 equilibration. PtGe/MCM-41 exhibited the higher selectivity than Pt/MCM-41 for the formation of ethylene in the hydrogenation of acetylene.





Zhiqiao He, Lei Xie, Shuang Song, Cheng Wang, Jinjun Tu, Fangyue Hong, Qi Liu, Jianmeng Chen, Xinhua Xu

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The impact of silver modification on the catalytic activity of iodine-doped titania for *p*-chlorophenol degradation under visible-light irradiation

Compared to I-TiO₂ and Ag-TiO₂, the photocatalytic activity of Ag-I-TiO₂ was enhanced markedly under visible-light irradiation owing to the synergistic effect of Ag and I. The PCP removal increased with increased Ag content up to 3% and then decreased, and the TOC that was used to prove the total mineralization of PCP had a similar trend.



Magdalena Hofman, Kotohiro Nomura

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1-Hexene polymerization by Cp*TiX₂(O-2,6- $^{i}Pr_{2}C_{6}H_{3})$ [X: Cl, Me] in the presence of MAO- and MMAOmodified carbonaceous supports 1-Hexene polymerization using Cp*TiX₂(O-2,6-iPr₂C₆H₃) (X = Cl, Me) in the presence of a series of MAO-, MMAO-modified (nitrogen enriched) carbonaceous materials have been conducted. The prepared carbonaceous supports were characterized by XPS method, and the catalytic activities were influenced by the nature of the supports employed, whereas the activity was not strongly affected by their surface areas.



K.M. Parida, Nruparaj Sahu, P. Mohapatra, M.S. Scurrell

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Gold (1 wt%) supported Fe–TiO₂ samples were prepared by varying iron content (1.0, 3.0, 5.0, 7.0 wt%). It was found that gold supported on the 5 wt% iron–titania sample gives 100% CO conversion at 80 °C, whereas gold titania gives only 7% at the same temperature.

 $\text{CO} + \text{O}_2 \xrightarrow[80]{\text{Au-5Fe-TiO}_2} \text{14 X Au-TiO}_2$

Low temperature CO oxidation over gold supported mesoporous $\mathrm{Fe-TiO}_2$

Sunyoung Park, Sung-Hyeon Baeck, Tae Jin Kim, Young-Min Chung, Seung-Hoon Oh, In Kyu Song

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Direct synthesis of hydrogen peroxide from hydrogen and oxygen over palladium catalyst supported on SO₃H-functionalized mesoporous silica Palladium catalysts supported on SO₃H-functionalized mesoporous silicas (Pd/SO₃H-MCM-41, Pd/SO₃H-MCM-48, Pd/SO₃H-MSU-1, Pd/SO₃H-SBA-15, and Pd/SO₃H-MCF) were applied to the direct synthesis of hydrogen peroxide from hydrogen and oxygen. Yield for hydrogen peroxide increased with increasing acid density of the catalyst. The catalysts efficiently served as an alternate acid source and as an active metal component in the reaction.



Alev Günyar, Fritz E. Kühn

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Bidentate Lewis base adducts of molybdenum(VI): Ligand impact on catalytic performance and stability Molybdenum(VI) complexes of the type MoO₂Cl₂ form adducts with bipyridine derivatives. The coordination of bidentate Lewis base ligands to Mo(VI) is governed by both electronic and steric effects due to the contributions of different functional groups on the bipyridine ligands. The bipyridine derived complexes show high catalytic activity and selectivity for cylooctene epoxidation.



Xiang Hui Liu, Hong Yan Song, Xiao Hua Ma, Martin J. Lear, Yu Zong Chen

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Virtual screening prediction of new potential organocatalysts for direct aldol reactions

A support vector machine (SVM) based virtual screening method is demonstrated as a rapid computational tool for the prediction of potential asymmetric organocatalysts for the direct aldol reaction. Our models show good accuracy at cross validation and independent testing. Structure analyses of screening hits from the PubChem database revealed several new classes of compounds, including β -amino acids, diamines and hydrazides, as potential chiral organocatalysts.



V.N. Panchenko, I. Borbáth, M.N. Timofeeva, S. Gőbölös

 $TBA_4HPW_{11}CoO_{39}$ chemically anchored to amino-modified silica ($NH_2-(CH_2)_x-SiO_2$, x = 0, 2, 3) was tested in $C_6H_5CH_2OH$ oxidation with O_2 . It was found that the higher the amount of anchored NH_2 -groups and the x value the higher the catalytic activity of immobilized $TBA_4HPW_{11}CoO_{39}$.

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Amine-modified silica $NH_2-(CH_2)_x-SiO_2$ (x = 0, 2, 3) as support for cobalt-substituted polyoxometalate TBA₄HPW₁₁CoO₃₉: Effect of the nature of the support on the oxidation activity

