Journal of Catalysis 270 (2010) iii–viii

Contents lists available at ScienceDirect

Journal of Catalysis

journal homepage: www.elsevier.com/locate/jcat

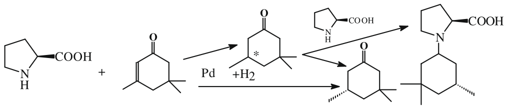
Journal of Catalysis Vol. 270, Issue 1, 2010

Contents

Editorial by Johannes Lercher .... **p 1**

Stereodifferentiation in heterogeneous catalytic hydrogenation. Kinetic resolution and asymmetric hydrogenation in the presence of (*S*)-proline: Catalyst-dependent processes **pp 2–8**

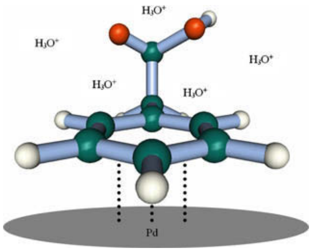
Nóra Győrffy*, Antal Tungler, Mátyás Fodor



Hydrogenation of dihydroisophorone (TMCH) and isophorone with (*S*)-proline over Pd catalysts was investigated. The optically active TMCH was formed not only by kinetic resolution but also through asymmetric C=C hydrogenation.

Aqueous phase hydrogenation of substituted phenyls over carbon nanofibre and activated carbon supported Pd **pp 9–15**

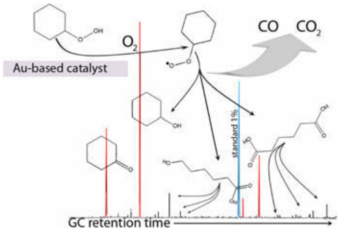
J.A. Anderson*, A. Athawale, F.E. Imrie, F.-M. M^c^Kenna, A. M^c^Cue, D. Molyneux, K. Power, M. Shand, R.P.K. Wells



Enhanced ring relative to functional group hydrogenation was induced using water as a solvent due to solvation of the polar functional group, which orientates the latter away from the surface.

Aerobic oxidation of cyclohexane by gold-based catalysts: New mechanistic insight by thorough product analysis **pp 16–25**

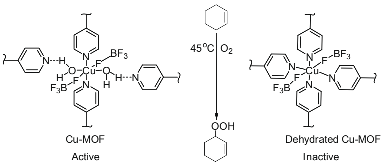
Bart P.C. Hereijgers, Bert M. Weckhuysen*



Through a detailed analysis of the product distribution during the catalytic oxidation of cyclohexane over Au-based catalysts, a radical-chain mechanism proceeding via peroxo-species was revealed.

Copper metal–organic framework: Structure and activity in the allylic oxidation of cyclohexene with molecular oxygen pp 26–33

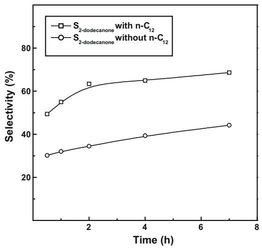
Dongmei Jiang, Tamas Mallat, Daniel M. Meier, Atsushi Urakawa, Alfons Baiker*



Cu(bpy)$(H_2O)_2(BF_4)_2$(bpy) (Cu-MOF) shows promising activity and high selectivity to allylic oxidation of cyclohexene with molecular oxygen under mild, solvent-free conditions. The reaction occurs at the surface of the latent porous framework and both bpy and water are involved in the active complex; removal of water opens the pores but eliminates the activity.

Oxidation of heavy 1-olefins ($C_{12}^{=} - C_{20}^{=}$) with TBHP using a modified Wacker system pp 34–39

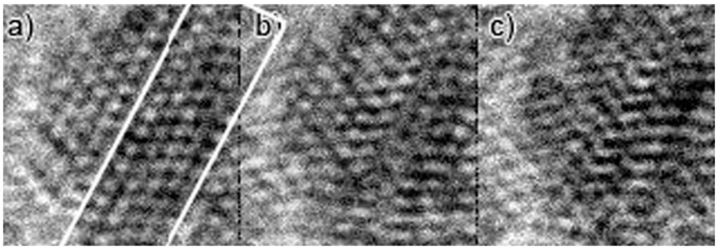
J.M. Escola*, J.A. Botas, C. Vargas, M. Bravo



The oxidation of heavy 1-olefins ($C_{12}^{=} - C_{20}^{=}$) was carried out using a modified Wacker system with TBHP as oxidant and acetonitrile as solvent at 80 °C. The presence of *n*-paraffins in the mixture increased the selectivity towards 2-methylketone due to a dilution effect which reduces the extent of the isomerisation reactions.

Mechanism of dynamic structural reorganization in polyoxometalate catalysts pp 40–47

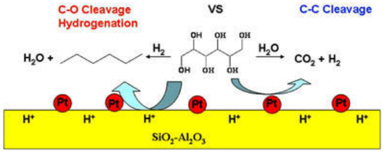
Hari Nair, Jeffrey T. Miller, Eric A. Stach, Chelsey D. Baertsch*



The molecular rearrangement of phosphomolybdic acid during thermal treatment is shown to occur through the formation and transmission of annealing twins responsible for its activation and deactivation when used as a catalyst for isobutane oxidation.

Aqueous-phase hydrodeoxygenation of sorbitol with $Pt/SiO_2–Al_2O_3$: Identification of reaction intermediates pp 48–59

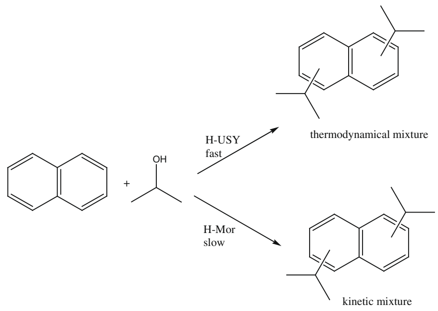
Ning Li, George W. Huber*



Reaction chemistry for the aqueous phase hydrodeoxygenation (APHDO) of sorbitol was studied over $Pt/SiO_2–Al_2O_3$ catalyst at 518 K and 2.93 MPa.

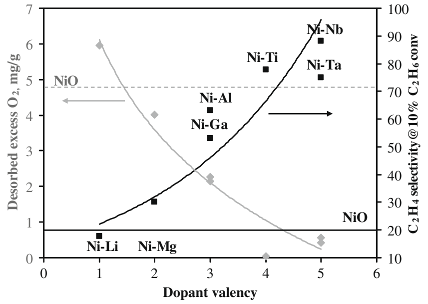
Shape-selective diisopropylation of naphthalene in H-Mordenite: Myth or reality? pp 60–66

Christophe Bouvier, Wim Buijs*, Jorge Gascon, Freek Kapteijn, Bogdan C. Gagea, Pierre A. Jacobs, Johan A. Martens



Ni–Me–O mixed metal oxides for the effective oxidative dehydrogenation of ethane to ethylene – Effect of promoting metal Me pp 67–75

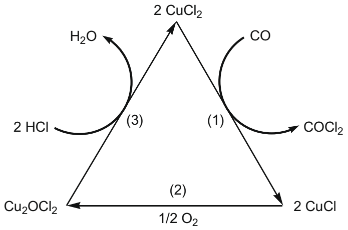
E. Heracleous*, A.A. Lemonidou



The study of Ni–Me–O with +1 to +5 valence metals demonstrated that based on the valence, dopants increase/decrease unselective excess oxygen of NiO, leading to reduced/enhanced activity in ethane ODH.

Oxychlorination of CO to phosgene in a three-step reaction cycle and corresponding catalytic mechanism pp 76–85

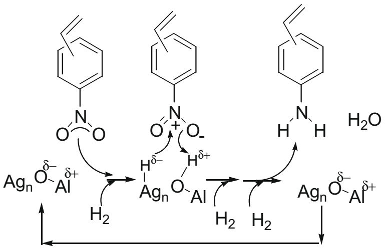
Tianzhu Zhang*, Carsten Troll, Bernhard Rieger*, Juergen Kintrup, Oliver F.-K. Schlüter, Rainer Weber



An important three-step reaction cycle for oxychlorination of CO to phosgene catalyzed by $CuCl_2$ was proposed, and the corresponding reaction mechanism was probed by the XRD measurements.

Size- and support-dependent silver cluster catalysis for chemoselective hydrogenation of nitroaromatics pp 86–94

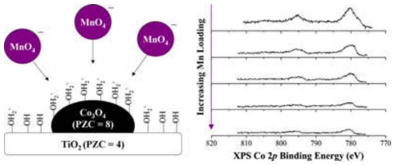
Ken-ichi Shimizu*, Yuji Miyamoto, Atsushi Satsuma



Chemoselective reduction of nitro group for the reduction of substituted nitroaromatics by silver–alumina proceeds by cooperation of coordinatively unsaturated Ag sites and acid–base sites of the support.

Selective adsorption of manganese onto cobalt for optimized Mn/Co/TiO$_2$ Fischer–Tropsch catalysts **pp 95–102**

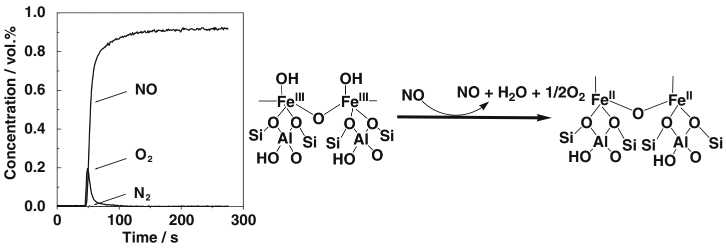
Theresa E. Feltes, Leticia Espinosa-Alonso, Emiel de Smit, Lawrence D'Souza, Randall J. Meyer, Bert M. Weckhuysen, John R. Regalbuto*



The preparation of a Mn-promoted Co/TiO$_2$ catalyst for Fischer–Tropsch synthesis was investigated using the Strong Electrostatic Adsorption method for deposition of Mn selectively onto Co to enhance promoter–metal interaction.

The promotional effect of NO on N$_2$O decomposition over the bi-nuclear Fe sites in Fe/ZSM-5 **pp 103–109**

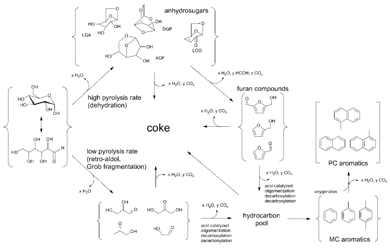
Haian Xia, Keqiang Sun, Zhimin Liu, Zhaochi Feng, Pinliang Ying, Can Li*



NO promotes the transformation of hydroxylated into active binuclear iron species of Fe/ZSM-5 at low temperatures.

Catalytic fast pyrolysis of glucose with HZSM-5: The combined homogeneous and heterogeneous reactions **pp 110–124**

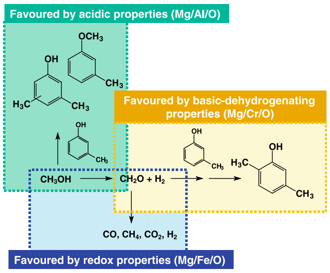
Torren R. Carlson, Jungho Jae, Yu-Chuan Lin, Geoffrey A. Tompsett, George W. Huber*



The homogeneous and heterogeneous chemistry for aromatic production from glucose in the presence of ZSM-5 catalyst was studied. We have identified the key intermediate species for aromatic production and coke formation and propose an overall reaction scheme for the direct conversion of glucose to aromatics.

The balance of acid, basic and redox sites in Mg/Me-mixed oxides: The effect on catalytic performance in the gas-phase alkylation of *m*-cresol with methanol **pp 125–135**

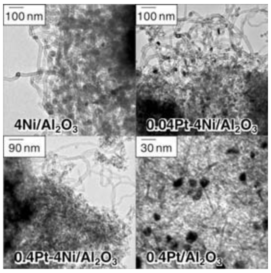
V. Crocellà, G. Cerrato, G. Magnacca, C. Morterra, F. Cavani*, S. Cocchi, S. Passeri, D. Scagliarini, C. Flego, C. Perego



Catalytic activity of Mg/Me (Me = Al^{3+}, Cr^{3+}, Fe^{3+})-mixed oxides in gas-phase methylation of phenol shows a pronounced dependence on the type of guest cation incorporated in MgO lattice.

Nanostructured Pt- and Ni-based catalysts for CO_2-reforming of methane pp 136–145

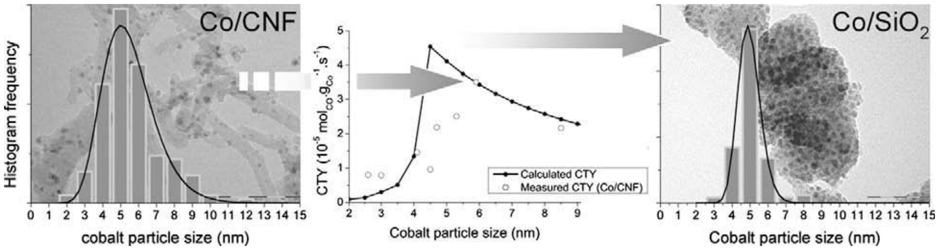
M. García-Diéguez, I.S. Pieta, M.C. Herrera, M.A. Larrubia, L.J. Alemany*



Pt–Ni catalysts supported on a novel nanofibrous alumina seems to be stable and selective catalysts for CO_2-reforming of methane.

Design of supported cobalt catalysts with maximum activity for the Fischer–Tropsch synthesis pp 146–152

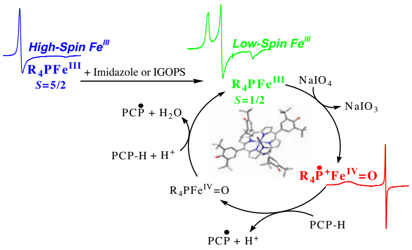
Johan P. den Breejen, Jelle R.A. Sietsma, Heiner Friedrich, Johannes H. Bitter, Krijn P. de Jong*



From TEM histograms and Fischer–Tropsch activities of Co/CNF catalysts, an optimum cobalt size with maximum activity was deduced. Based on this knowledge, a highly active Co/SiO_2 catalyst with a narrow size distribution was synthesized.

Mechanism of catalytic decomposition of pentachlorophenol by a highly recyclable heterogeneous SiO_2–[Fe-porphyrin] catalyst pp 153–162

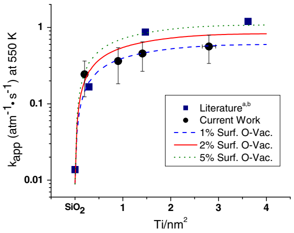
Konstantinos C. Christoforidis, Maria Louloudi, Elena R. Milaeva, Yiannis Deligiannakis*



Efficient catalytic decomposition of PCP is achieved by a highly recyclable heterogenized $FeR_4P–SiO_2$ catalyst. The catalytic reactive intermediate $R_4P^+Fe^{IV}O$ has been detected by EPR and DR-UV–Vis specrsocpy in the heterogeneous phase.

An experimental and theoretical investigation of the structure and reactivity of bilayered $VO_x/TiO_x/SiO_2$ catalysts for methanol oxidation pp 163–171

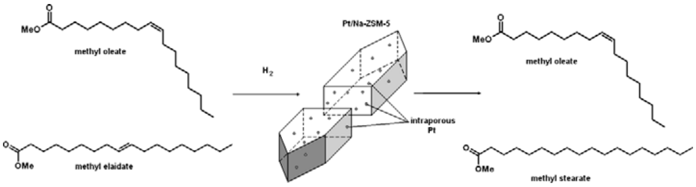
William C. Vining, Anthony Goodrow, Jennifer Strunk, Alexis T. Bell*



A bilayered $VO_x/TiO_x/SiO_2$ catalyst consisting of vanadia deposited onto silica containing a submonolayer of titania was studied using both experiment and theory. The catalyst was shown to consist of isolated V atoms with VOSi and VOTi bonds. A theoretical model using absolute rate theory and quantum chemical calculations models both the reaction rate and activation energy.

Selectivity in sorption and hydrogenation of methyl oleate and elaidate on MFI zeolites pp 172–184

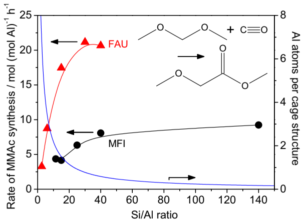
An Philippaerts, Sabine Paulussen, Stuart Turner, Oleg I. Lebedev, Gustaaf Van Tendeloo, Hilde Poelman, Metin Bulut, Filip De Clippel, Pieter Smeets, Bert Sels*, Pierre Jacobs*



Selective catalytic removal of *trans*-monounsaturated fatty acid methyl esters: nano-sized Pt clusters embedded within Na–ZSM-5 zeolite crystals preferentially catalyze the hydrogenation of methyl elaidate (*trans* isomer) from its equimolar mixture with methyl oleate (*cis* isomer).

Effect of zeolite framework type and Si/Al ratio on dimethoxymethane carbonylation pp 185–195

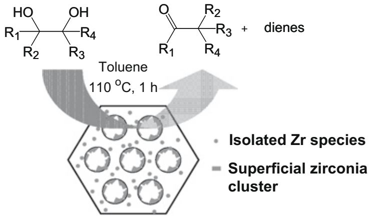
Fuat E. Celik, Tae-Jin Kim, Alexis T. Bell*



The role of zeolite structure and composition in the carbonylation of dimethoxymethane to methyl methoxyacetate was investigated at steady state. Faujasite (FAU) showed higher selectivity than medium-pore zeolites such as ZSM-5 (MFI). Carbonylation rates increased with increasing Si/Al ratio until one or fewer Al atoms were located in the supercage of FAU or the channel intersections of MFI.

Pinacol-type rearrangement catalyzed by Zr-incorporated SBA-15 pp 196–205

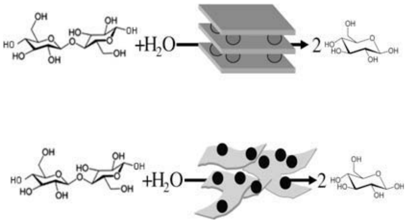
Shih-Yuan Chen, Jyh-Fu Lee, Soofin Cheng*



One-pot synthesized Zr–SBA-15 materials containing superficial zirconia clusters were the most efficient catalyst in pinacol-type rearrangement, in comparison with ZSM-5 and HY-zeolites, as well as impregnated ZrO_2/SBA-15 materials.

Layered and nanosheet tantalum molybdate as strong solid acid catalysts pp 206–212

Caio Tagusagawa, Atsushi Takagaki, Kazuhiro Takanabe, Kohki Ebitani, Shigenobu Hayashi, Kazunari Domen*



Layered and nanosheet aggregates of $HTaMoO_6$ were found as highly active solid acid catalysts for Friedel–Crafts alkylation and hydrolysis reactions due to intercalation behavior and strong acid sites on the layers.