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Articles

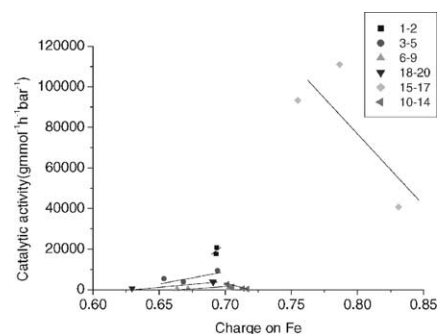
Tianzhu Zhang, Wen-Hua Sun, Ting Li, Xiaozhen Yang

Journal of Molecular Catalysis A: Chemical 218 (2004) 119

Influence of electronic effect on catalytic activity of bis(imino)pyridyl Fe(II) and bis(imino)pyrimidyl Fe(II) complexes

The metal atom net charge correlation (MANCC) was successfully used to study the relative catalytic activities of 20 bis(imino)pyridyl Fe(II) and bis(imino)pyrimidyl Fe(II) complexes for olefins polymerization/oligomerization through modifying the Dreiding force. The net charge range on the central metal Fe was found 0.6295–0.8310, which was considered in the present study as two areas, e.g. the lower charge area (0.6295–0.7000) and the higher charge area (0.7000–0.8310). The observations reveal that the catalytic activity of bis(imino)pyridyl Fe(II) and bis(imino)pyrimidyl Fe(II) complexes does not monotonously vary with the net charge on the central metal as we found for other metal system before. There possibly is an interesting turning point around 0.7000. The activity increases with the net charge in the

lower charge area, while the catalytic activity increases with reducing the net charge in the higher area. The reason that the Fe(II) catalysts possess such properties was discussed.

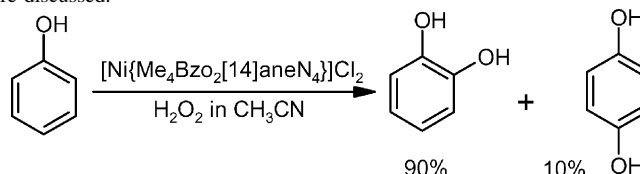


Hanna S. Abbo, Salam J.J. Titinchi, Shri Chand, Rajendra Prasad

Journal of Molecular Catalysis A: Chemical 218 (2004) 125

Investigation of [Ni{Me₄Bzo₂[14]aneN₄}]Cl₂ catalyzed selective hydroxylation of phenol to catechol by H₂O₂ in the homogeneous medium

The nickel(II) macrocycle complex catalyzed selective oxidation of phenol to catechol by H₂O₂ with an over all efficiency of >40% under homogeneous conditions. The electrochemical and chemical catalysis parameters are discussed.

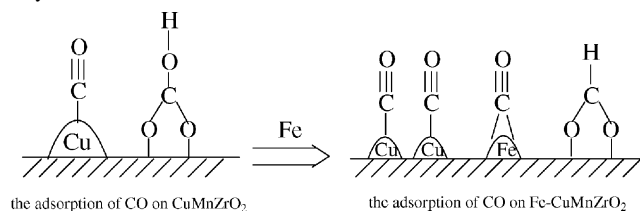


Run Xu, Zhong-yi Ma, Cheng Yang, Wei Wei, Wen-huai Li, Yu-han Sun

Journal of Molecular Catalysis A: Chemical 218 (2004) 133

The effect of iron on the adsorption properties of CuMnZrO₂ catalysts studied by temperature-programmed desorption and FTIR spectroscopy

When iron was introduced in CuMnZrO₂ catalyst, it was found that the adsorption features of catalysts changed significantly. The presence of iron improved the copper dispersion, which resulted in the total adsorption of CO increase, and intensified the reaction between CO and catalyst surface. Moreover, the CO bridge-adsorbed on iron sites was detected. Bicarbonate species formed on the CuMnZrO₂ catalyst when CO adsorption took place at 573 K, while formate species were favored and predominant on the Fe-CuMnZrO₂ catalyst.

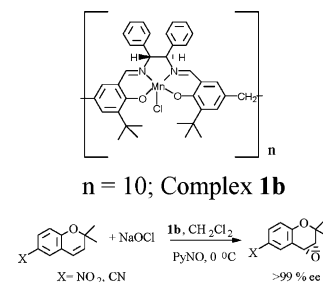


**Rukhsana I. Kureshy, Noor-ul H. Khan,
Sayed H.R. Abdi, Surendra Singh,
Irshad Ahmed, Raksh V. Jasra**

Journal of Molecular Catalysis A: Chemical 218
(2004) 141

Catalytic asymmetric epoxidation of non-functionalised alkenes using polymeric Mn(III) Salen as catalysts and NaOCl as oxidant

Enantioselective epoxidation of non-functionalised alkenes using polymeric Mn(III) Salen complex in presence of PyN–O using NaOCl gave excellent (>99%) epoxide yield with high chiral induction in case of nitro and cyano chromene and the catalyst could be reused up to five cycles.

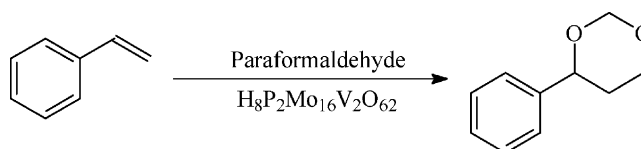


**Guixian Li, Yanlong Gu, Yong Ding,
Hanpeng Zhang, Jianming Wang,
Qiang Gao, Liang Yan, Jishuan Suo**

Journal of Molecular Catalysis A: Chemical 218
(2004) 147

Wells–Dawson type molybdovanadophosphoric heteropolyacids catalyzed Prins cyclization of alkenes with paraformaldehyde under mild conditions—a facile and efficient method to 1,3-dioxane derivatives

Wells–Dawson type molybdovanadophosphoric heteropolyacids ($\text{H}_{6+n}\text{P}_2\text{Mo}_{18-n}\text{V}_n\text{O}_{62}$) ($n = 1-2, 4$) have proved to be effective catalysts for Prins cyclization between alkenes and paraformaldehyde to produce corresponding 1,3-dioxane derivatives.

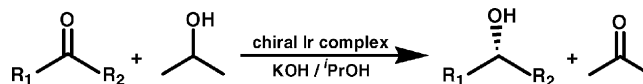


**Yan-Yun Li, Hui Zhang, Jian-Shan Chen,
Xin-Li Liao, Zhen-Rong Dong, Jing-Xing Gao**

Journal of Molecular Catalysis A: Chemical 218
(2004) 153

A new efficient chiral iridium catalyst for asymmetric transfer hydrogenation of ketones

A new chiral diaminodiphosphine-Ir(I) complex was prepared and applied to catalytic asymmetric transfer hydrogenation of various aromatic ketones with up to 99.0% ee.

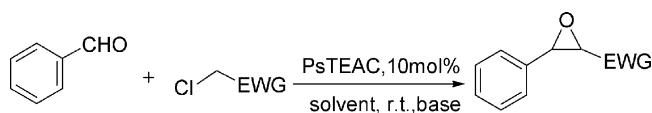


**Zongting Wang, Liwen Xu, Zonggang Mu,
Chungu Xia, Hanqing Wang**

Journal of Molecular Catalysis A: Chemical 218
(2004) 157

Efficient Darzens condensation reactions of aromatic aldehydes catalyzed by polystyrene-supported phase-transfer catalyst

The Darzens reaction of α -chloroester and nitrile with aromatic aldehydes under mild conditions proceeds in the presence of polystyrene-supported quaternary ammonium salt (polystyrene-supported triethylammonium chloride, Ps-TEAC) as phase-transfer catalyst (PTC) to give the corresponding cis- and trans-desired products in satisfactory yields.

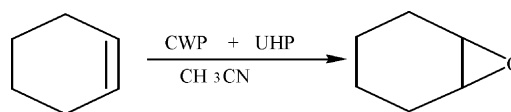


**Yong Ding, Qiang Gao, Guixian Li,
Hanpeng Zhang, Jianmin Wang, Liang Yan,
Jishuan Suo**

Journal of Molecular Catalysis A: Chemical 218
(2004) 161

Selective epoxidation of cyclohexene to cyclohexene oxide catalyzed by Keggin-type heteropoly compounds using anhydrous urea–hydrogen peroxide as oxidizing reagent and acetonitrile as the solvent

The epoxidation of cyclohexene catalyzed by Keggin-type heteropoly compounds (HPAs) were investigated using anhydrous urea–hydrogen peroxide adduct (UHP) as an oxidant and acetonitrile as a solvent. Among a series of Keggin-type heteropoly compounds, tris(cetylpyridinium)12-tungstophosphate (CWP) showed the highest activity.

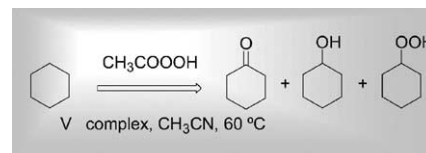


**Laura Gonzalez Cuervo, Yuriy N. Kozlov,
Georg Süß-Fink, Georgiy B. Shul'pin**

Journal of Molecular Catalysis A: Chemical 218
(2004) 171

Oxidation of saturated hydrocarbons with peroxyacetic acid catalyzed by vanadium complexes

Vanadium(V) and vanadium(IV) complexes catalyze oxidation of various alkanes with peroxyacetic acid to produce corresponding alcohols, ketones and alkyl hydroperoxides.

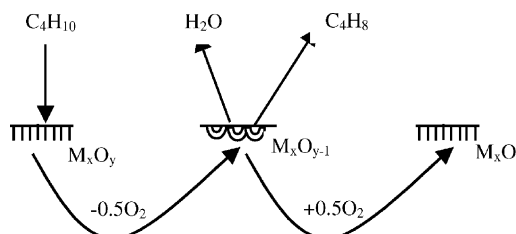


**S.M. Al-Zahrani, N.O. Elbashir,
A.E. Abasaheed, M. Abdulwahed**

Journal of Molecular Catalysis A: Chemical 218
(2004) 179

Isobutane oxydehydrogenation on Al₂O₃-supported transition and rare-earth metal oxides

Oxidative dehydrogenation of isobutane to isobutene was carried out using, as catalysts, some transition and rare-earth metals supported on Al₂O₃. Below 400 °C, Cr gave the best performance (10% conversion and 62% selectivity) while above 500 °C, Ni showed the highest activity (32% conversion).



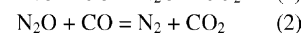
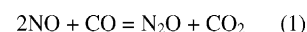
**Jiang Xiaoyuan, Ding Guanghui, Lou Liping,
Chen Yingxu, Zheng Xiaoming**

Journal of Molecular Catalysis A: Chemical 218
(2004) 187

Catalytic activities of CuO/TiO₂ and CuO-ZrO₂/TiO₂ in NO + CO reaction

The catalytic activities were improved dramatically compared with treatment in normal air at 500 °C for 2 h. The NO conversion temperature ($T_{99\%}$) was 325 °C for 6% CuO/TiO₂ and 300 °C for 6% CuO-10% ZrO₂/TiO₂, and their activities increased with increase in ZrO₂ loading. During the thermal desorption of NO, there were four desorption species (NO, N₂O, N₂ and O₂) for CuO/TiO₂ and CuO-ZrO₂/TiO₂ treated in both air and H₂. There were two adsorption states of NO on the catalyst's surface, i.e. desorption species at low temperature on the weak sites and at high temperature on the strong sites. Addition of ZrO₂ onto CuO/TiO₂ shifted the NO dissociation

peaks towards low temperature, which means that the activity of NO decomposition was higher by CuO-ZrO₂/TiO₂ than by CuO/TiO₂. The overall reaction schemes involved in NO + CO reaction can be summarized as the followings:

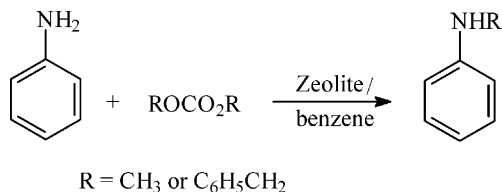


**Thirugnanasamy Esakkidurai,
Kasi Pitchumani**

Journal of Molecular Catalysis A: Chemical 218
(2004) 197

Zeolite-promoted selective mono-*N*-methylation
of aniline with dimethyl carbonate

Selective mono-*N*-methylation of aniline with dimethyl carbonate is carried out over faujasite Y zeolites. Benzylation with dibenzyl carbonate is also found to be very selective, resulting in exclusive mono-benylation. Other advantages such as lower temperature, less rigorous reaction conditions, absence of C-alkylation products, etc., are also highlighted.

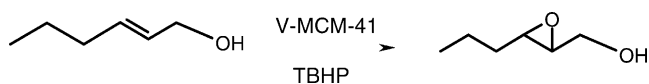


F. Farzaneh, E. Zamanifar, Craig D. Williams

Journal of Molecular Catalysis A: Chemical 218
(2004) 203

V-MCM-41 as selective catalyst for epoxidation of
olefins and *trans*-2-hexene-1-ol

V-MCM-41 has been synthesized by one pot synthesis. The oxidation of olefins such as 1-hexene, cyclohexene, cyclopentene, norbornene and *trans*-2-hexene-1-ol with TBHP in the presence of V-MCM-41 in different solvents (acetone, acetonitrile, dichloromethane, chloroform) is described.

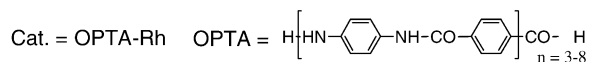
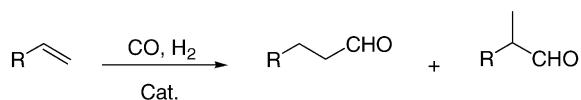


G. Cum, P. Famulari, M. Marchetti, B. Sechi

Journal of Molecular Catalysis A: Chemical 218
(2004) 211

Hydroformylation by rhodium catalysts supported
on oligomeric arylamides

Hydroformylation of various unsaturated substrates has been carried out using an oligomeric complex obtained by adding Rh(CO)₂(acac) to oligo-1,4-phenyleneterephthalamide (OPTA). The reaction performed at 80 °C and 80 atm (CO/H₂ = 1:1), in autoclave using an innovative glass device gave satisfactory results. The catalyst was easily recycled and could be reused 8–9 times without significant loss of efficiency.

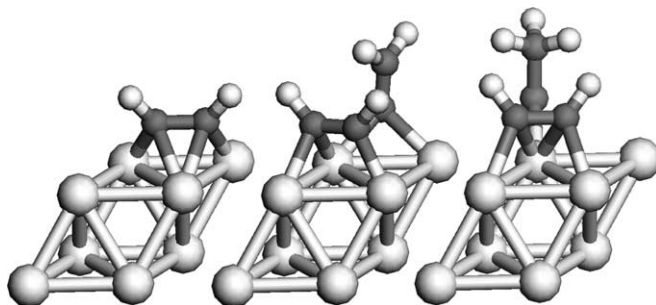


**Simon G. Podkolzin, Rafael Alcalá,
James A. Dumesic**

Journal of Molecular Catalysis A: Chemical 218
(2004) 217

Density functional theory studies of acetylene
hydrogenation on clean, vinylidene- and ethylidyne-covered Pt(1 1 1) surfaces

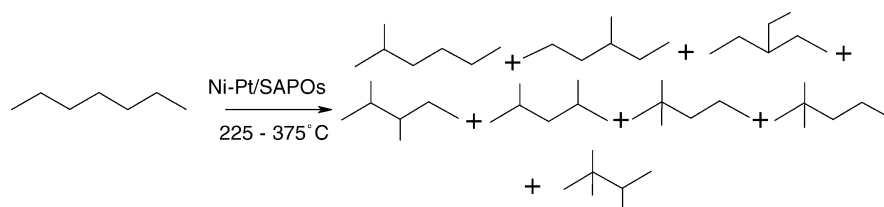
Density functional theory (DFT) calculations were carried out to study the stability and reactivity of various hydrocarbon intermediates involved in acetylene hydrogenation on Pt(1 1 1) in the presence of vinylidene and ethylidyne species. These latter species can also alter the activity and selectivity for acetylene hydrogenation by participating in hydrogen transfer reactions.



I. Eswaramoorthi, N. Lingappan

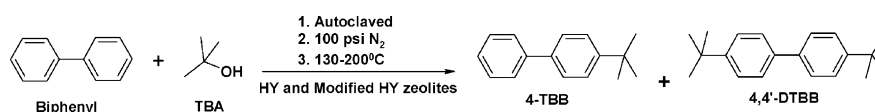
Journal of Molecular Catalysis A: Chemical 218 (2004) 229

Ni-Pt loaded silicoaluminophosphate molecular sieves for hydroisomerisation of n-heptane


R. Anand, S.S. Khaire, R. Maheswari, K.U. Gore

Journal of Molecular Catalysis A: Chemical 218 (2004) 241

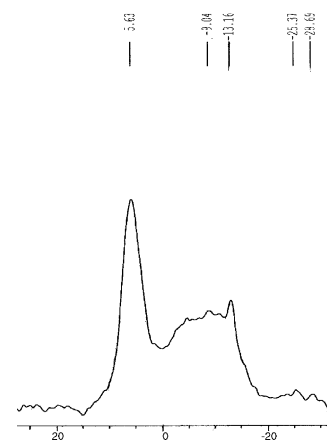
Alkylation of biphenyl with *t*-butylalcohol over modified Y zeolites


Jian Li, Shuang Gao, Meng Li, Ronghua Zhang, Zuwei Xi

Journal of Molecular Catalysis A: Chemical 218 (2004) 247

Influence of composition of heteropolyphosphatungstate catalyst on epoxidation of propylene

A series of heteropolyphosphatungstate catalysts with different structure were tested for the propylene epoxidation reaction. The structure entity at ca. $\delta = 5$ ppm in ^{31}P MAS NMR spectra is very probably a catalyst precursor which can be the most efficiently converted to $\{\text{PO}_4[\text{WO}(\text{O}_2)_2]_4\}^{3-}$.


Xinbin Ma, Jinlong Gong, Shengping Wang, Fei He, Xia Yang, Gang Wang, Genhui Xu

Journal of Molecular Catalysis A: Chemical 218 (2004) 253

Characterization and reactivity of silica-supported bimetallic molybdenum and stannic oxides for the transesterification of dimethyl oxalate with phenol

XRD spectra of supported monometallic oxide and supported bimetallic MoSn oxide catalysts with different Mo(Sn) loadings, B₁: 8%Mo; B₂: 8%Sn; C₁: 1%Mo-1%Sn; C₂: 2%Mo-2%Sn; C₃: 4%Mo-4%Sn; C₄: 6%Mo-6%Sn; C₅: 8%Mo-8%Sn; C₆: 10%Mo-10%Sn; C₇: 12%Mo-12%Sn; C₈: 14%Mo-14%Sn; C₉: 16%Mo-16%Sn. The appearance of tetragonal crystal SnO₂ phase strengthened the promotional effect of Sn and led to the increase in the activity of supported bimetallic MoO₃-SnO₂/SiO₂ catalysts.

