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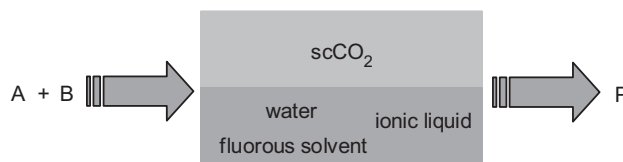
Articles

Shifang Liu, Jianliang Xiao

Journal of Molecular Catalysis A: Chemical 270 (2007) 1

Toward green catalytic synthesis—Transition metal-catalyzed reactions in non-conventional media

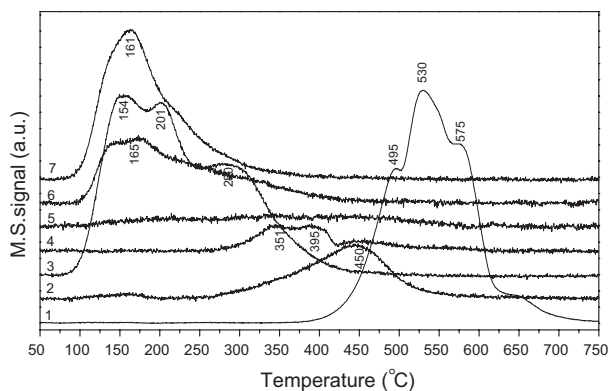
A review is presented on catalysis in water, ionic liquids, supercritical CO₂ and fluorous solvents, highlighting the progress made in the past few years.



Qibiao Li, Ning Zhao, Wei Wei, Yuhuan Sun

Journal of Molecular Catalysis A: Chemical 270 (2007) 44

Catalytic performance of metal oxides for the synthesis of propylene carbonate from urea and 1,2-propanediol

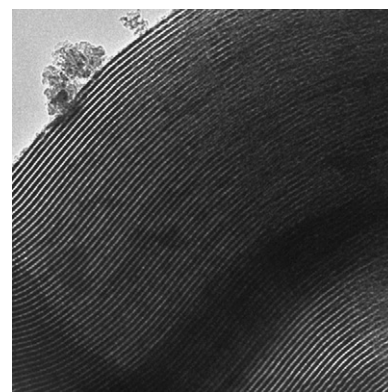


Yan Zhou, Renlie Bao, Bin Yue, Min Gu, Supeng Pei, Heyong He

Journal of Molecular Catalysis A: Chemical 270 (2007) 50

Synthesis, characterization and catalytic application of SBA-15 immobilized rare earth metal sandwiched polyoxometalates

Rare earth metal sandwiched Keggin-type heteropolyoxometalates, K₁₁[RE(PW₁₁O₃₉)₂] (RE = La, Ce, Pr, Nd, Sm, Eu, Dy and Y), were immobilized onto aminosilylated mesoporous silica SBA-15. The samples show higher catalytic efficiency than the bulk ones in heterogeneous epoxidation of cyclohexene with H₂O₂. The leaching of active species is negligible and the recycled catalysts retain high activity.

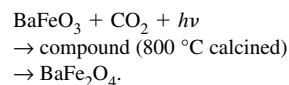


**Yang Yang, Yinshan Jiang, Yingwei Wang,
Yanbin Sun**

Journal of Molecular Catalysis A: Chemical 270
(2007) 56

Photoinduced decomposition of BaFeO₃ during
photodegradation of methyl orange

Photocatalyst BaFeO₃ has been synthesized by the citrate–nitrate combustion method. The photocatalytic activity of BaFeO₃ has been evaluated for photodegradation of methyl orange under UV light irradiation. Structural information of BaFeO₃ obtained by X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy, X-ray photoelectron spectroscopy (XPS) indicates that the valence state of iron ions in BaFeO₃ changes after the photocatalytic experiment and discussed.

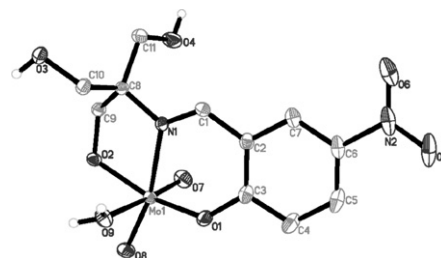


**Yan Sui, Xirui Zeng, Xiaoniu Fang,
Xiangkai Fu, Yi'an Xiao, Li Chen, Menghua Li,
Shu Cheng**

Journal of Molecular Catalysis A: Chemical 270
(2007) 61

Syntheses, structure, redox and catalytic epoxidation
properties of dioxomolybdenum(VI) complexes
with Schiff base ligands derived from tris(hydrox-
methyl)amino methane

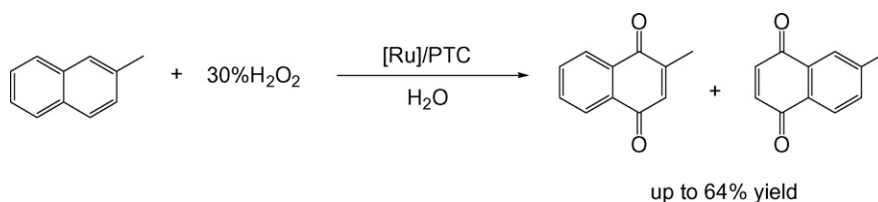
Five kinds of dioxomolybdenum(VI) complexes
with Schiff base ligands derived from tris(hydrox-
methyl)amino methane are prepared and struc-
turally characterized. These complexes are found to
be effective catalysts in the epoxidation of cyclo-
hexene with *t*-butylhydroperoxide, especially for **4**,
which could give a nearly 100% of conversion and
selectivity. The substituents in the salicylidene ring
strongly influence the redox stability and catalytic
effectiveness.



Feng Shi, Man Kin Tse, Matthias Beller

Journal of Molecular Catalysis A: Chemical 270
(2007) 68

Selective oxidation of naphthalene derivatives with
ruthenium catalysts using hydrogen peroxide as
terminal oxidant

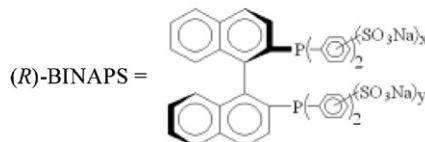
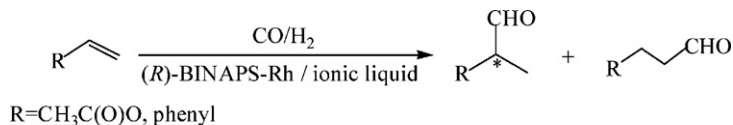


**Changxi Deng, Guangnan Ou, Jiarong She,
Youzhu Yuan**

Journal of Molecular Catalysis A: Chemical 270
(2007) 76

Biphasic asymmetric hydroformylation and hydro-
genation by water-soluble rhodium and ruthenium
complexes of sulfonated (*R*)-2,2'-bis(diphenylphos-
phino)-1,1'-binaphthyl in ionic liquids

Biphasic catalytic systems with water-soluble rhodium and ruthenium complexes of sulfonated (*R*)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl ((*R*)-BINAPS) in ionic liquid have been developed for the asymmetric hydroformylation and hydrogenation under mild conditions. The biphasic catalytic systems with (*R*)-BINAPS ligand could be reused several times without significantly reducing the activity, enantio- and regio-selectivities.

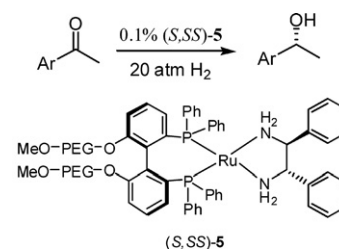


Li-Ting Chai, Wei-Wei Wang, Quan-Rui Wang, Feng-Gang Tao

Journal of Molecular Catalysis A: Chemical 270 (2007) 83

Asymmetric hydrogenation of aromatic ketones with MeO-PEG-supported BIPHEP/DPEN ruthenium catalysts

The soluble MeO-PEG-supported BIPHEP-Ru/chiral diamine (DPEN) complex **5** was prepared, and employed as catalyst for asymmetric hydrogenation of various aromatic ketones, providing comparable or even higher enantioselectivity than that achieved with BINAP-Ru-DPEN catalyst under similar conditions. The catalyst showed good recoverability, and could be used for five consecutive runs without a significant drop in enantioselectivity.

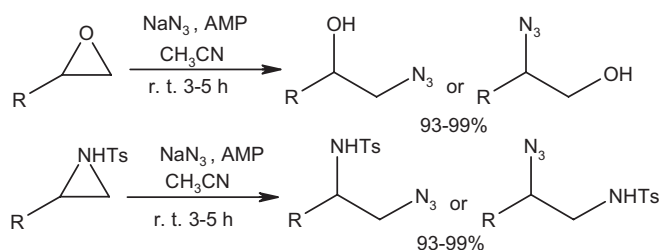


Ar = (substituted)phenyl, 3-pyridyl, thiophen-2-yl, 1-naphthyl

Biswanath Das, Vtukuri Saidi Reddy, Maddeboina Krishnaiah, Yerra Koteswara Rao

Journal of Molecular Catalysis A: Chemical 270 (2007) 89

Highly regio- and stereoselective ring-opening of epoxides and aziridines with sodium azide using ammonium-12-molybdophosphate

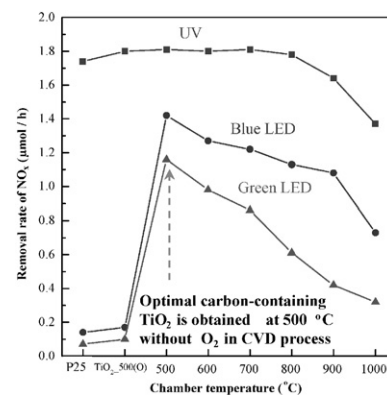


Chien-Sheng Kuo, Yao-Hsuan Tseng, Chia-Hung Huang, Yuan-Yao Li

Journal of Molecular Catalysis A: Chemical 270 (2007) 93

Carbon-containing nano-titania prepared by chemical vapor deposition and its visible-light-responsive photocatalytic activity

A thermal decomposition reaction of titanium isopropoxide was conducted to synthesize the visible-light-responsive titania under the metal-organic chemical vapor deposition process. Carbon-containing titania with the anatase phase prepared at 500 °C under oxygen free atmosphere exhibited a high photocatalytic activity for the oxidation of NO under visible light. The carbonaceous species on the TiO₂ was supposed to be an important factor for the visible-light response.

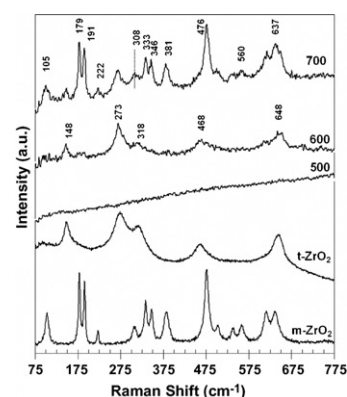


Erik M. Holmgren, Matthew M. Yung, Umit S. Ozkan

Journal of Molecular Catalysis A: Chemical 270 (2007) 101

Pd-based sulfated zirconia prepared by a single step sol-gel procedure for lean NO_x reduction

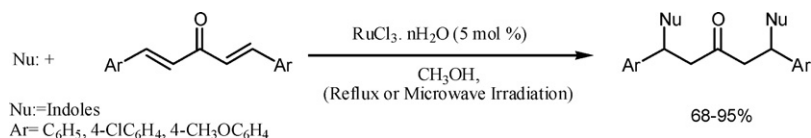
Pd/sulfated zirconia catalysts were prepared through a single step sol-gel procedure. The catalysts were active for the reduction of NO₂ with CH₄ under lean conditions. Higher calcinations temperatures resulted in more active catalysts, corresponding to support phase changes and differences in the observed surface sulfate species. This figure shows Raman spectra revealing changes in the surface zirconia phase at different calcination temperatures.



**K. Tabatabaieian, M. Mamaghani,
N.O. Mahmoodi, A. Khorshidi**

Journal of Molecular Catalysis A: Chemical 270
(2007) 112

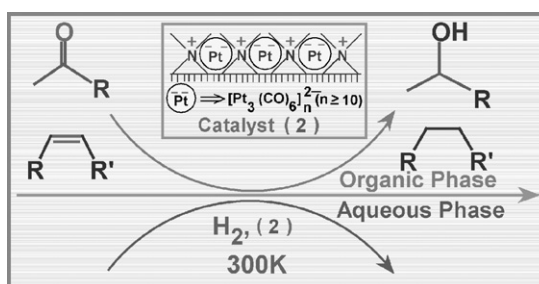
Ru^{III}-catalyzed double-conjugate 1,4-addition of
indoles to symmetric enones



**Prasenjit Maity, Susmit Basu, Sumit Bhaduri,
Goutam Kumar Lahiri**

Journal of Molecular Catalysis A: Chemical 270
(2007) 117

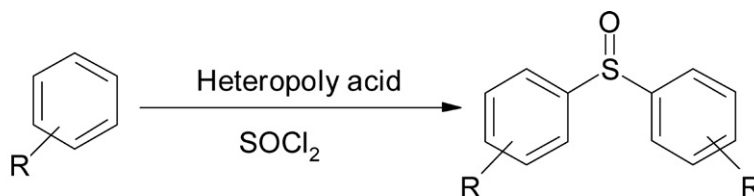
A water soluble nanostructured platinum (0) metal
catalyst from platinum carbonyl molecular clusters:
Synthesis, characterization and application in the
selective hydrogenations of olefins, ketones and
aldehydes



**Sachin V. Bhilare, Amol R. Deorukhkar,
Nitin B. Darvatkar, Meghana S. Rasalkar,
Manikrao M. Salunkhe**

Journal of Molecular Catalysis A: Chemical 270
(2007) 123

An efficient and direct route to the synthesis of
diaryl sulfoxides catalyzed by heteropoly acid

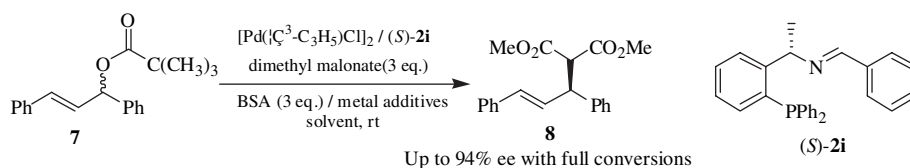


Heteropoly acid catalyzed synthesis of symmetrical diaryl sulfoxides

**Jia-Di Huang, Xiang-Ping Hu, Sai-Bo Yu,
Jun Deng, Dao-Yong Wang, Zheng-Chao Duan,
Zhuo Zheng**

Journal of Molecular Catalysis A: Chemical 270
(2007) 127

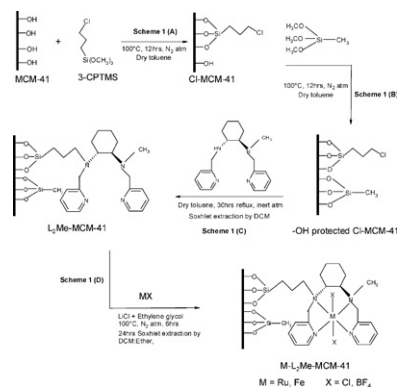
Readily available phosphine-imine ligands from α -
phenylethylamine for highly efficient Pd-catalyzed
asymmetric allylic alkylation



Tamijselvy Soundiressane, S. Selvakumar,
Stéphane Ménage, Olivier Hamelin,
Marc Fontecave, Anand P. Singh

Journal of Molecular Catalysis A: Chemical 270
(2007) 132

Ru- and Fe-based *N,N'*-bis(2-pyridylmethyl)-*N*-methyl-(1*S*,2*S*)-1,2-cyclohexanediamine complexes immobilised on mesoporous MCM-41: Synthesis, characterization and catalytic applications



Abhishek Sud, Raj M. Deshpande,
Raghunath V. Chaudhari

Journal of Molecular Catalysis A: Chemical 270
(2007) 144

Kinetics of vinylation of 4'-bromoacetophenone with *n*-butyl acrylate using palladacycle catalyst

The kinetics of vinylation of 4'-bromoacetophenone with *n*-butyl acrylate has been studied using palladacycle catalyst precursor **1**, in the presence of NaOAc as a base and tetrabutylammonium bromide as a promoter in *N*-methyl-2-pyrrolidinone as solvent. The rate of reaction was found to be first order with respect to 4'-BAP, half order with the catalyst, and first order tending to zero with NaOAc concentration. The rates passed through a maximum with variation of TBAB and *n*-butyl acrylate concentrations. The rate data have been analyzed to propose an empirical model, which is consistent with the mechanism already established for Heck reactions.



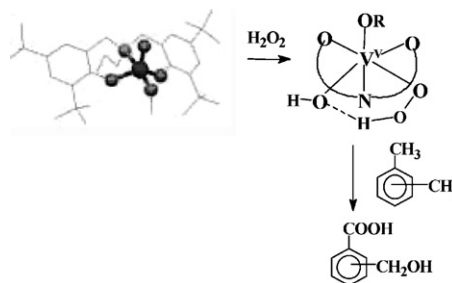
$$R = \frac{k[4\text{'-BAP}][n\text{-BA}][\text{NaOAc}][\text{TBAB}][\text{Cat}]^{0.5}}{(1 + K_{n\text{-BA}}[n\text{-BA}]^2)(1 + K_{\text{NaOAc}}[\text{NaOAc}])(1 + K_{\text{TBAB}}[\text{TBAB}]^2)}$$

Dipankar Maity, Jaromir Marek,
W.S. Sheldrick, H. Mayer-Figge,
Mahammad Ali

Journal of Molecular Catalysis A: Chemical 270
(2007) 153

Synthesis, crystal structures and catalytic oxidation of aromatic hydrocarbons by oxovanadium(V) complexes of aminebis(phenolate) ligands

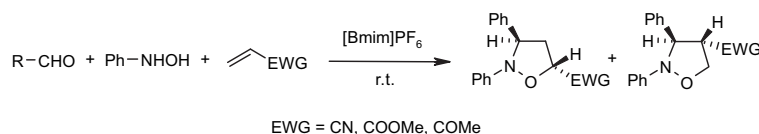
Three VHPO model complexes have been characterized by single crystal X-ray structure analysis and were found to catalyze the oxidation of toluene to benzoic acid and isomers of xylenes to the corresponding hydroxy acids with turn over numbers ranging between 134 and 188 where hydroxo-hydroperoxy species acts as an active intermediate.



J.S. Yadav, B.V.S. Reddy, P. Sreedhar,
Ch.V.S.R. Murthy, G. Mahesh, G. Kondaji,
K. Nagaiah

Journal of Molecular Catalysis A: Chemical 270
(2007) 160

Three-component coupling reactions in ionic liquids: One-pot synthesis of isoxazolidines

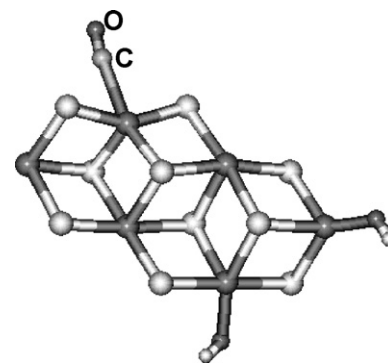


Dmitry A. Trubitsyn, Vladimir A. Zakharov, Ivan I. Zakharov

Journal of Molecular Catalysis A: Chemical 270 (2007) 164

A theoretical investigation of the adsorption surface sites of the activated MgCl_2

The adsorption of carbon monoxide on activated MgCl_2 has been investigated within DFT using different models of the MgCl_2 surface. It has been found that proposed model based on the geometry of the relaxed MgCl_2 surface allows to simulate the IR bands of the adsorbed CO within the accuracy better than 10 cm^{-1} . A new model of the adsorption surface sites of the activated MgCl_2 .

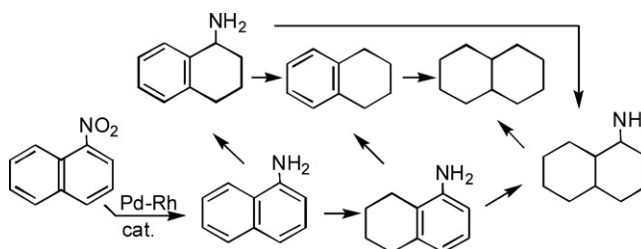


Tatiana Tehila Bovkun, Michael Grayevsky, Yoel Sasson, Jochanan Blum

Journal of Molecular Catalysis A: Chemical 270 (2007) 171

Liquid phase hydrogenation and hydrodenitrogenation of aromatic nitrogen-containing environmental pollutants

In the presence of a silica sol-gel entrapped catalyst composed of metallic palladium and $[\text{Rh}(\text{cod})(\mu\text{-Cl})_2]$ under 27.6 bar H_2 at 80–140 °C carcinogenic nitro- and amino-polycyclic aromatic hydrocarbons are hydrodenitrogenated. Using 1-nitronaphthalene as a model compound, it was found that initially the nitro-compounds are reduced to mixtures of primary and secondary amines that ultimately form polycyclic alicyclic hydrocarbons and ammonia.

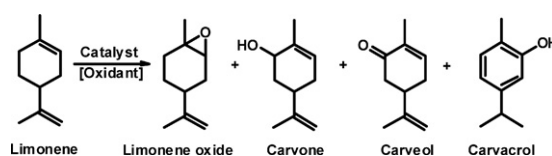


Ankur Bordoloi, F. Lefebvre, S.B. Halligudi

Journal of Molecular Catalysis A: Chemical 270 (2007) 177

Organotin-oxometalate coordination polymer catalyzed oxyfunctionalization of monoterpenes

The organotin-oxometalate coordination polymers $[(n\text{Bu}_3\text{Sn})_2\text{MO}_4] \cdot n\text{H}_2\text{O}$, (where, M = Mo or W) were tested in oxyfunctionalization of monoterpenes such as limonene, α -pinene, β -pinene, carene, camphene, gerrniol and linalool with urea hydroperoxide (UHP) as an oxidizing agent in acetonitrile solvent to give high epoxide selectivities of monoterpenes.

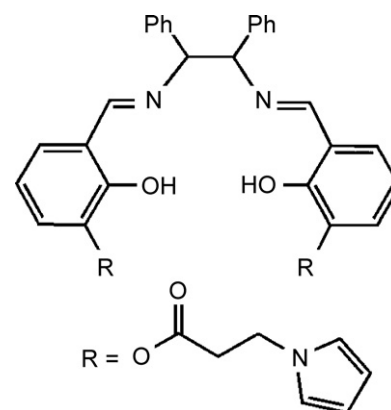


Sofia M. Bruno, Saete S. Balula, Anabela A. Valente, Filipe A. Almeida Paz, Martyn Pillinger, Carla Sousa, Jacek Klinowski, Cristina Freire, Paulo Ribeiro-Claro, Isabel S. Gonçalves

Journal of Molecular Catalysis A: Chemical 270 (2007) 185

Synthesis and catalytic properties in olefin epoxidation of dioxomolybdenum(VI) complexes bearing a bidentate or tetradentate *salen*-type ligand

The molybdenum complexes $[\text{MoO}_2(\text{oep-saldpen})]$ and $[\text{MoO}_2\text{Cl}_2(\text{oep-H}_2\text{saldpen})]$, with a tetradentate $[\text{N}_2(\text{imine})\text{O}_2]$ and bidentate $[\text{N}_2(\text{imine})]$ *salen*-type ligand, respectively, were prepared and characterised by ^1H NMR, IR and Raman spectroscopy. The complexes were examined as catalysts for the epoxidation of cyclooctene, (*R*)-(+)-limonene, styrene, α -pinene, and *cis* and *trans*- β -methylstyrene, with *tert*-butyl hydroperoxide. Both complexes exhibit high selectivity for the epoxidation reaction, with the bis(chloro) complex being always the more active catalyst.

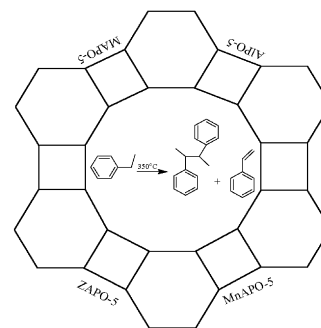


**K. Joseph Antony Raj, M.S. Meenakshi,
V.R. Vijayaraghavan**

Journal of Molecular Catalysis A: Chemical 270
(2007) 195

Ethylation and disproportionation of ethylbenzene over substituted AFI type molecular sieves

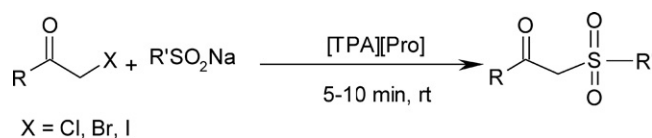
The vapour and liquid phase ethylation of ethylbenzene performed over AFI type molecular sieves. The results of vapour phase reactions show a faster deactivation of the catalyst due to temperatures at which the reactions performed. The liquid phase reactions showed a higher selectivity for *para*-diethylbenzene (84.4%) than the vapour phase reaction. When ethylbenzene passed over MnAPO-5, yielded styrene and 2,3-diphenylbutane. This showed a preference for oxidation rather than disproportionation followed by alkylation.



**N. Suryakiran, P. Prabhakar, K. Rajesh,
V. Suresh, Y. Venkateswarlu**

Journal of Molecular Catalysis A: Chemical 270
(2007) 201

Synthesis of β -keto-sulfones using ionic liquid [TPA][Pro] as an efficient and reusable reaction medium

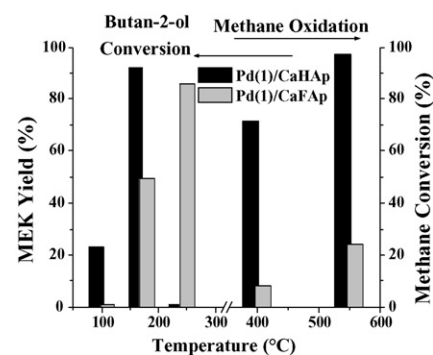


**Zouhair Boukha, Mohamed Kacimi,
Mahfoud Ziyad, Alain Ensueque,
François Bozon-Verduraz**

Journal of Molecular Catalysis A: Chemical 270
(2007) 205

Comparative study of catalytic activity of Pd loaded hydroxyapatite and fluoroapatite in butan-2-ol conversion and methane oxidation

Fluorination of hydroxyapatite CaHAp has a marked effect on the catalytic behaviour of supported palladium: (i) in dehydrogenation of butan-2-ol to MEK, Pd/CaHAp is more efficient than Pd/CaFAp below 180 °C and active in *butan-2-ol combustion* above 180 °C whereas Pd/CaFAp is not; (ii) in methane combustion, Pd/CaHAp is much more active than Pd/CaFAp. These differences are related to PdO particle size, larger on Pd/CaFAp, and to differences in surface acidity.

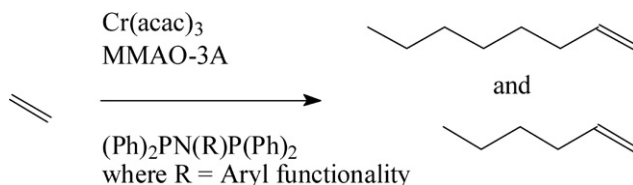


**Esna Killian, Kevin Blann, Annette Bollmann,
John T. Dixon, Sven Kuhlmann,
Munaka C. Maumela, Hulisani Maumela,
David H. Morgan, Palesa Nongodlwana,
Matthew J. Overett, Marié Pretorius,
Karola Höfener, Peter Wasserscheid**

Journal of Molecular Catalysis A: Chemical 270
(2007) 214

The use of bis(diphenylphosphino)amines with *N*-aryl functionalities in selective ethylene tri- and tetramerisation

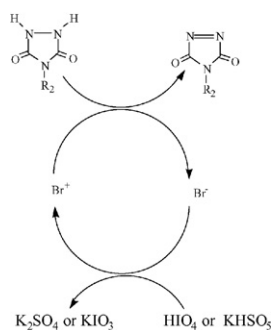
A systematic study was conducted on the Cr catalysed tri- and tetramerisation of ethylene using bis(diphenylphosphino)amine ligands with *N*-aryl functionality. This study revealed that the oligomerisation reaction product selectivity is primarily dependent on the structure and size of this family of *N*-aryl groups.



Mohammad Ali Zolfigol, Mojtaba Bagherzadeh, Shadpour Mallakpour, Gholamabbas Chehardoli, Arash Ghorbani-Choghamarani, Nadiya Koukabi, Mina Dehghanian, Mahmoudreza Doroudgar

Journal of Molecular Catalysis A: Chemical 270 (2007) 219

The first report on the catalytic oxidation of urazoles to their corresponding triazolinediones via *in situ* catalytic generation of Br^+ using periodic acid or oxone[®]/KBr system

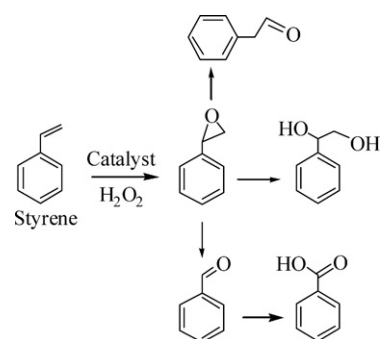


Mannar R. Maurya, Anil K. Chandrakar, Shri Chand

Journal of Molecular Catalysis A: Chemical 270 (2007) 225

Oxovanadium(IV) and copper(II) complexes of 1,2-diaminocyclohexane based ligand encapsulated in zeolite-Y for the catalytic oxidation of styrene, cyclohexene and cyclohexane

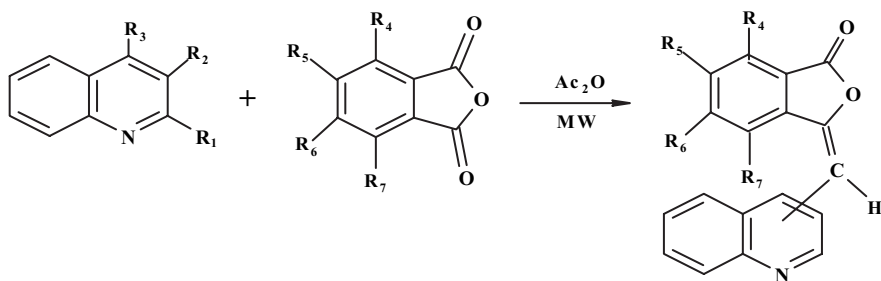
Oxovanadium(IV) and copper(II) complexes of Schiff bases derived from salicylaldehyde and 1,2-diaminocyclohexane have been encapsulated in the cavity of zeolite-Y and characterized. These complexes catalyse the oxidation, by peroxide, of styrene cyclohexene and cyclohexane in good yield.



Javad Safari, Hossein Naeimi, Ali Akbar Khakpour, Ramezan Sharifi Jondani, Shiva Dehghan Khalili

Journal of Molecular Catalysis A: Chemical 270 (2007) 236

A rapid and efficient method for synthesis of new 3-arylideneisobenzofuran-1(3H)-one derivatives catalyzed by acetic anhydride under solvent-free and microwave conditions

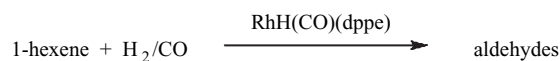


Merlin Rosales, Angel González, Yusbeli Guerrero, Inés Pacheco, Roberto A. Sánchez-Delgado

Journal of Molecular Catalysis A: Chemical 270 (2007) 241

Kinetics and mechanisms of homogeneous catalytic reactions. Part 7. Hydroformylation of 1-hexene catalyzed by cationic complexes of rhodium and iridium containing PPH

The kinetics and mechanism of 1-hexene hydroformylation were studied using $\text{Rh}(\text{acac})(\text{CO})_2/\text{dppe}$ as catalyst at 80 °C, 1–7 atm H_2 and 1–7 atm CO in toluene. $\text{RhH}(\text{CO})(\text{dppe})$ is the active species, hydrogenolysis of the acyl intermediate is rate-determining at low H_2 pressure, while olefin insertion into the Rh-H bond is rate-limiting at high H_2 pressure.

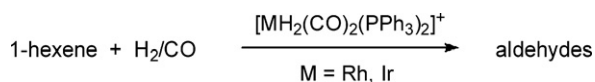


**Merlin Rosales, Jesús A. Durán,
Ángel González, Inés Pacheco,
Roberto A. Sánchez-Delgado**

Journal of Molecular Catalysis A: Chemical 270
(2007) 250

Kinetics and mechanisms of homogeneous catalytic reactions

The kinetics and mechanism of 1-hexene hydroformylation were studied using $[M(\text{COD})(\text{PPh}_3)_2]\text{PF}_6$, $M = \text{Rh}, \text{Ir}$ as catalyst precursors at 60–100 °C, 2–5 atm H_2/CO in toluene. For both complexes, the reaction proceeds according to the rate law $r_1 = K_1 K_2 K_3 [\text{M}][\text{olef}][\text{H}_2][\text{CO}] / ([\text{CO}]^2 + K_1 [\text{H}_2][\text{CO}] + K_1 K_2 [\text{olef}][\text{H}_2])$ and a catalytic cycle is proposed involving hydride transfer to the alkene as the rds.

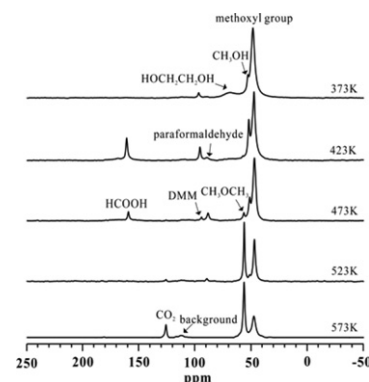


**Danlin Zeng, Hanjun Fang, Anmin Zheng,
Jun Xu, Lei Chen, Jun Yang, Jiqing Wang,
Chaohui Ye, Feng Deng**

Journal of Molecular Catalysis A: Chemical 270
(2007) 257

Selective oxidation of methanol over supported vanadium oxide catalysts as studied by solid-state NMR spectroscopy

Solid-state NMR spectroscopy results show that stronger acid sites in $\text{VO}_x/\text{Al}_2\text{O}_3$ lead to almost the same selectivities for dimethoxymethane (DMM), paraformaldehyde and formic acid, and weaker acid sites in VO_x/ZrO_2 favor paraformaldehyde synthesis, while the VO_x/MgO catalyst with base support shows high selectivity for formate. ^{13}C single-pulse MAS NMR spectra (with proton decoupling) of methanol and oxygen reaction on $\text{VO}_x/\text{Al}_2\text{O}_3$ at various temperatures.

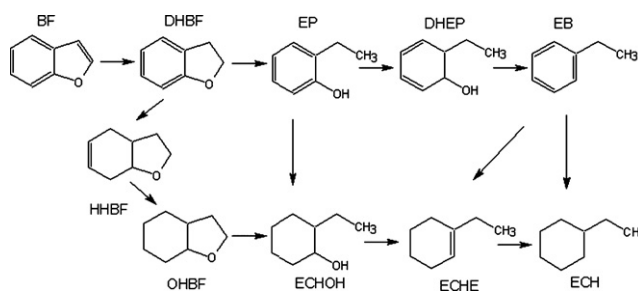


Abdu Y. Bunch, Xueqin Wang, Umit S. Ozkan

Journal of Molecular Catalysis A: Chemical 270
(2007) 264

Hydrodeoxygenation of benzofuran over sulfided and reduced $\text{Ni-Mo}/\gamma\text{-Al}_2\text{O}_3$ catalysts: Effect of H_2S

Effect of H_2S on the catalytic performance of the reduced and sulfided $\text{Ni-Mo}/\text{Al}_2\text{O}_3$ catalysts in hydrodeoxygenation of benzofuran is studied. A change in product distribution is observed due to a change in the relative abundance of hydrogenation and hydrogenolysis sites, which promote different routes in the reaction scheme shown in the figure.

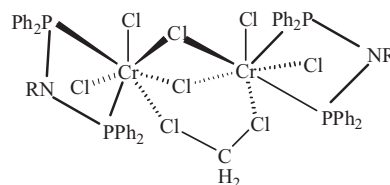


**Hongxia Chen, Xiaoyu Liu, Wenbo Hu,
Yingnan Ning, Tao Jiang**

Journal of Molecular Catalysis A: Chemical 270
(2007) 273

Effects of halide in homogeneous $\text{Cr}(\text{III})/\text{PNP}/\text{MAO}$ catalytic systems for ethylene tetramerization toward 1-octene

The possible coordination structures of halide with chromium center are shown here. In the interaction mode, geminal chloro groups act as two-point weak Lewis base sites which fit with two Cr sites of dimeric $\text{Cr}(\text{III})/\text{PNP}$ complex. The specific interaction mode between dimeric $\text{Cr}(\text{III})/\text{PNP}$ complex and geminal chloro groups is expected to stabilize the active center.



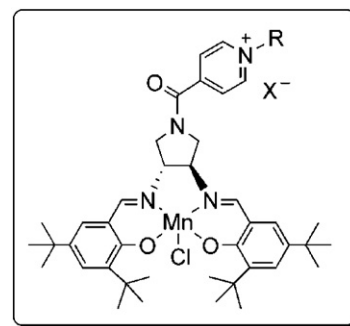
Possible interaction modes between geminal chloro groups and dimeric $\text{Cr}(\text{III})$.

**Dongping Wang, Mei Wang, Xiuna Wang,
Rong Zhang, Jia Ma, Licheng Sun**

Journal of Molecular Catalysis A: Chemical 270 (2007) 278

Influence of the built-in pyridinium salt on asymmetric epoxidation of substituted chromenes catalysed by chiral (pyrrolidine salen)Mn(III) complexes

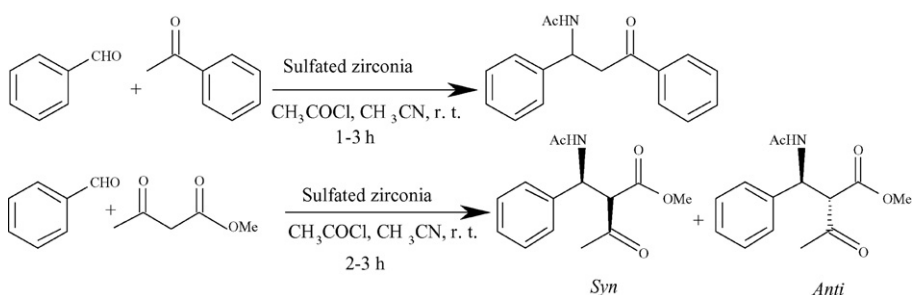
The (pyrrolidine salen)Mn(III) complexes with an internal pyridinium salt displayed considerably higher activities than their analogous complexes and Jacobsen's catalyst for asymmetric epoxidation of chromenes in the aqueous/organic biphasic medium, with comparable high yields and ee values. The acceleration of the reaction rate is attributed to the phase transfer capability of the built-in pyridinium salt of the (salen)Mn(III) catalyst.



**Biswanath Das, Maddeboina Krishnaiah,
Keetha Laxminarayana, K. Ravinder Reddy**

Journal of Molecular Catalysis A: Chemical 270 (2007) 284

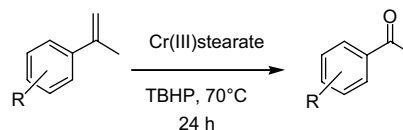
A simple and efficient one-pot synthesis of β -acetamido carbonyl compounds using sulfated zirconia as a heterogeneous recyclable catalyst



**Suekanya Jarupinthusophon,
Uthumporn Thong-In, Warinthorn Chavasiri**

Journal of Molecular Catalysis A: Chemical 270 (2007) 289

Catalytic oxidative cleavage of terminal olefins by chromium(III) stearate



**Mohamed Elanany, Bao-Lian Su,
Daniel P. Vercauteren**

Journal of Molecular Catalysis A: Chemical 270 (2007) 295

Strong templating effect of TEAOH in the hydrothermal genesis of the $\text{AlPO}_4\text{-5}$ molecular sieve: Experimental and computational investigations

Monitoring the hydrothermal genesis of $\text{AlPO}_4\text{-5}$ by means of XRD and DFT calculations shows that TEAOH has the best templating effect toward the formation of $\text{AlPO}_4\text{-5}$ structure from the synthesis gels among the investigated organic templates series, viz., MCHA, TEA, TPA, and TEAOH.

