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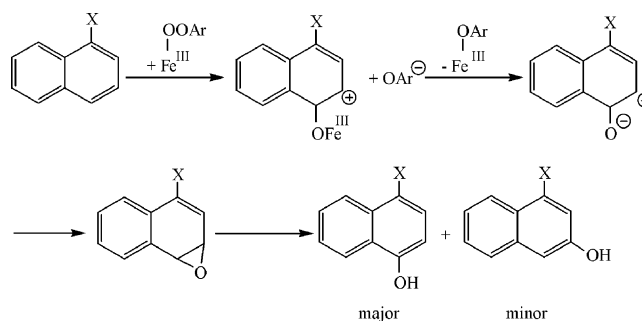
Articles

Hamid Reza Khavasi, Nasser Safari

Journal of Molecular Catalysis A: Chemical 220 (2004) 127

Model reaction related to cytochrome P-450: effect of substitution on the rate of naphthalene oxidation

The relative rates of naphthalene hydroxylation were determined by a competitive kinetic method. Based upon oxidation potentials, Hammett and Hammett–Brown plots versus $\log k_{rel}$ and oxidation products, a mechanism including peroxy iron intermediate was proposed.



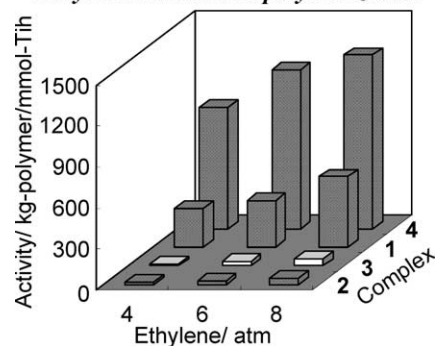
Kotohiro Nomura, Kazuya Fujita, Michiya Fujiki

Journal of Molecular Catalysis A: Chemical 220 (2004) 133

Olefin polymerization by (cyclopentadienyl)(ketimide)titanium(IV) complexes of the type, $Cp'TiCl_2(N=C'Bu_2)$ -methylaluminoxane (MAO) catalyst systems

(Cyclopentadienyl)(ketimide)titanium complexes of type, $Cp'TiCl_2(N=C'Bu_2)$ [$Cp' = Cp$ (**1**), $tBuCp$ (**2**), Cp^* (**3**), indenyl (**4**)], exhibited significant catalytic activities for ethylene/1-hexene copolymerization, and the activities increased in the order: $4 > 1 \gg 2, 3$. The r_E/r_H values by **1–3** were 0.35–0.52, indicating that the 1-hexene incorporation did not proceed in a random manner: the r_E values were independent upon Cp' but increased at higher temperature.

Ethylene/1-hexene copolymerization

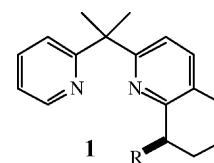


Giorgio Chelucci, Simona Chessa, Gianmauro Orrù

Journal of Molecular Catalysis A: Chemical 220 (2004) 145

Application of chiral dipyriddy methane ligands in the enantioselective palladium-catalyzed allylic alkylation

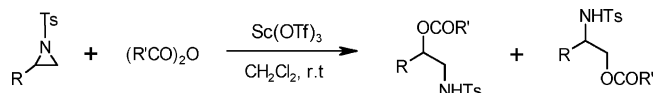
New chiral C_1 -symmetric dipyriddy methane ligands with general formula **1** have been prepared and assessed in the enantioselective palladium catalyzed allylic alkylation of 1,3-diphenylprop-2-enyl acetate with dimethylmalonate. Enantioselectivity up to 68% ee has been obtained.



**J.S. Yadav, B.V.S. Reddy, K. Sadashiv,
K. Harikishan, A.V. Narsaiah**

Journal of Molecular Catalysis A: Chemical 220
(2004) 153

Acylative cleavage of aziridines with acid anhydrides catalyzed by Scandium triflate

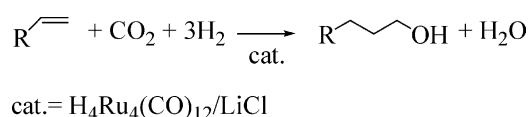


Ken-ichi Tominaga, Yoshiyuki Sasaki

Journal of Molecular Catalysis A: Chemical 220
(2004) 159

Ruthenium-catalyzed one-pot hydroformylation of alkenes using carbon dioxide as a reactant

Various alkenes were hydroformylated with carbon dioxide to give the corresponding alcohols in the presence of ruthenium cluster complexes and chloride salts. This reaction was found to be catalyzed by combination of tetra- and mononuclear ruthenium species.



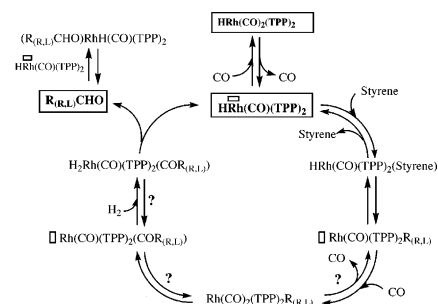
C. Bergounhou, D. Neibecker, R. Mathieu

Journal of Molecular Catalysis A: Chemical 220
(2004) 167

Kinetics and mechanism of the hydroformylation of styrene catalysed by the rhodium/TPP system (TPP = 1,2,5-triphenyl-1H-phosphole)

A kinetic study of the hydroformylation of styrene catalysed by the rhodium/TPP (1,3,5-triphenyl-1H-phosphole) system is presented. The catalytic system is shown to involve an active species bearing two TPP ligands, which remain coordinated to the metal throughout the catalytic cycle. The proposed mechanistic model involves the formation of an adduct between a styrene molecule and the unsaturated species $\text{HRh}(\text{CO})(\text{TPP})_2$. An analytical equation of the reaction rate is established. The selectivity between linear and branched alkyl-rhodium derivatives appears to be under thermodynamic control. The aldehydes which are produced throughout the reaction are shown to exert an inhibiting effect reflecting their tendency to coordinate back to the metal. Subtle

effects of CO and hydrogen partial pressures on the reaction rate are also emphasized.

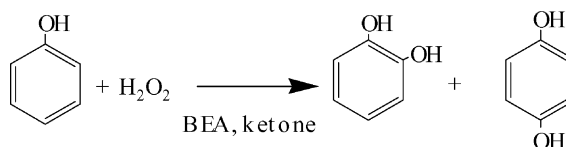


**Takashi Atoguchi, Tomonori Kanougi,
Toshio Yamamoto, Shigeru Yao**

Journal of Molecular Catalysis A: Chemical 220
(2004) 183

Phenol oxidation into catechol and hydroquinone over H-MFI, H-MOR, H-USY and H-BEA in the presence of ketone

Effective catalytic combination of H-BEA zeolite and ketone for phenol oxidation with hydrogen peroxide was obtained.

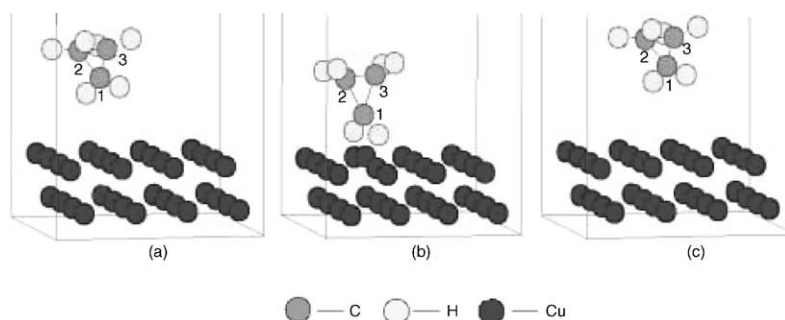


**Xiaoqing Wang, Parasuraman Selvam,
Chen Lv, Momoji Kubo, Akira Miyamoto**

Journal of Molecular Catalysis A: Chemical 220
(2004) 189

A theoretical study on the cyclopropane adsorption onto the copper surfaces by density functional theory and quantum chemical molecular dynamics methods

A theoretical study of cyclopropane adsorption onto Cu(111) surfaces was performed by density functional theory (DFT). Moreover, the dynamic adsorption process was simulated using our novel accelerated quantum chemical molecular dynamics program 'Colors' as shown in the figure.

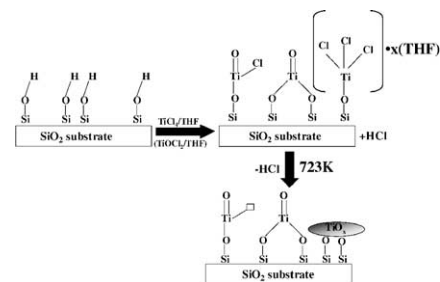


**Spyridon Ntais, Vassilios Dracopoulos,
Angeliki Siokou**

Journal of Molecular Catalysis A: Chemical 220
(2004) 199

TiCl₄(THF)₂ impregnation on a flat SiO_x/Si(1 0 0) and on polycrystalline Au foil: determination of surface species using XPS

The interaction of TiCl₄(THF)₂ with a flat SiO_x layer and a Au foil was studied at 300 K and after annealing at 723 K by XPS and AFM. A mixed Si:O:Ti interfacial layer was formed on the silicon substrate while TiOCl_x and TiO_x were the main surface species on Au at 300 K. At 723 K, total desorption of the Cl occurs in both cases and a homogenous distribution of nano-sized TiO_x clusters is observed on the SiO_x/Si(1 0 0) substrate.

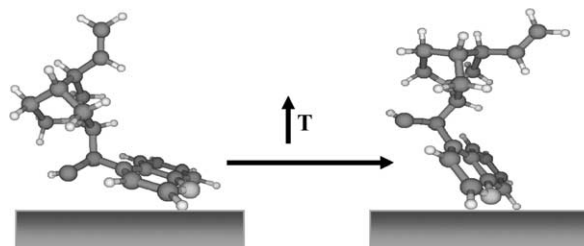


Rene J. LeBlanc, Christopher T. Williams

Journal of Molecular Catalysis A: Chemical 220
(2004) 207

Surface Raman characterization of cinchonidine-modified polycrystalline platinum in ethanol: effects of temperature and comparison with 10,11-dihydrocinchonidine

Surface-enhanced Raman spectroscopy has been utilized to probe the adsorption of the chiral modifier cinchonidine on platinum in ethanol over the temperature range 30–70 °C. The changes observed on cinchonidine-modified Pt above 40 °C include a significant tilting of the aromatic quinoline group of cinchonidine with respect to the surface. The observed behavior correlates well with reported decreases in enantioselectivity and turn-over frequency at similar temperatures during the ethyl pyruvate hydrogenation reaction.

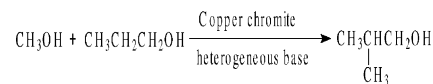


**Carlo Carlini, Cristina Flego,
Mario Marchionna, Marilena Noviello,
Anna Maria Raspolli Galletti, Glauco Sbrana,
Francesco Basile, Angelo Vaccari**

Journal of Molecular Catalysis A: Chemical 220
(2004) 215

Guerbet condensation of methanol with *n*-propanol to isobutyl alcohol over heterogeneous copper chromite/Mg–Al mixed oxides catalysts

The catalytic synthesis of isobutyl alcohol via the Guerbet condensation of methanol with *n*-propanol, has been studied. Two-component catalysts based on pre-activated copper chromite, as heterogeneous dehydrogenating/hydrogenating metal-containing species, and a heterogeneous base consisting of Mg/Al mixed oxides derived from hydrotalcite precursors with different Mg/Al atomic ratios, were investigated.

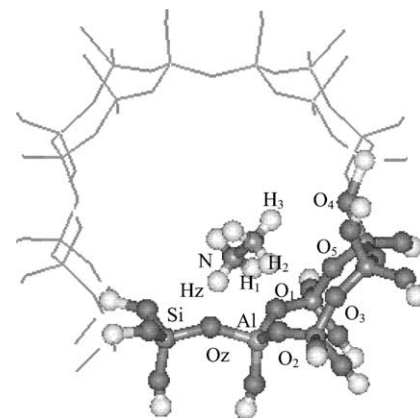


**Nan Jiang, Shuping Yuan, Jianguo Wang,
Haijun Jiao, Zhangfeng Qin, Yong-Wang Li**

Journal of Molecular Catalysis A: Chemical 220
(2004) 221

A theoretical study of amines adsorption in HMOR by using ONIOM2 method

The adsorption of amines (NH_3 , MeNH_2 , Me_2NH and Me_3N) in H-type mordenite (HMOR) is investigated by using ONIOM2 method. Proton transfer is found between HMOR and the amines with the formation of $[\text{HNR}_3]^+$, which is stabilized by the hydrogen bonding between the hydrogens of amines and the lattice oxygens of the zeolite substrate. On the basis of the calculated adsorption energies, the relative basicity of amines in HMOR has the order of $\text{NH}_3 < \text{MeNH}_2 < \text{Me}_3\text{N} < \text{Me}_2\text{NH}$.

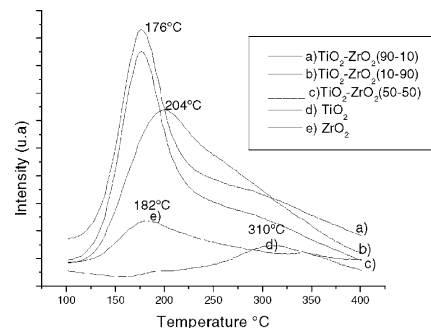


**M.E. Manríquez, T. López, R. Gómez,
J. Navarrete**

Journal of Molecular Catalysis A: Chemical 220
(2004) 229

Preparation of TiO_2 - ZrO_2 mixed oxides with controlled acid-basic properties

Ammonia TPD profiles for TiO_2 , ZrO_2 and TiO_2 - ZrO_2 catalysts showing medium strength acid sites in the mixed oxides.

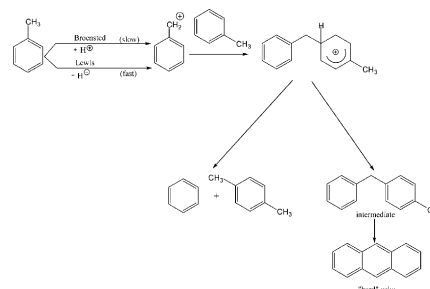


**V. Mavrodinova, M. Popova, R.M. Mihályi,
G. Pál-Borbély, Ch. Minchev**

Journal of Molecular Catalysis A: Chemical 220
(2004) 239

Toluene disproportionation and coking on zeolites Y modified with Lewis-connected InO^+ acid sites

The effect of introduction of Lewis acid sites on the reactions of toluene transformation and catalysts coking has been studied over parent ($\text{Si}/\text{Al} = 2.5$) and dealuminated ($\text{Si}/\text{Al} = 3.7$) Y zeolites modified with Lewis connected InO^+ cationic acid sites. A relation has been found between the initially accelerated processes of alkyl transfer and the reinforced formation of carbonaceous deposits over the In-modified catalysts.

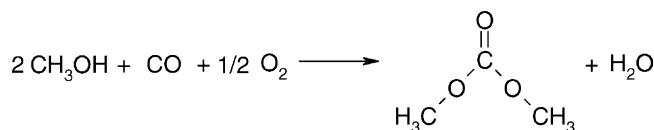


Steven A. Anderson, Thatcher W. Root

Journal of Molecular Catalysis A: Chemical 220
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Investigation of the effect of carbon monoxide on the oxidative carbonylation of methanol to dimethyl carbonate over Cu^+X and $\text{Cu}^+\text{ZSM-5}$ zeolites

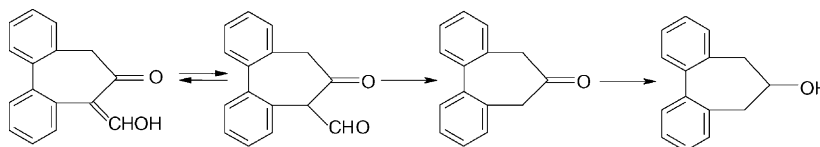
Direct synthesis of dimethyl carbonate (DMC) as a 'Green Chemistry' replacement for phosgene depends strongly on competitive adsorption of reactants over different supported copper zeolites.



**Simona M. Coman, Anca Dobre,
Mircea D. Banciu, Aurica Petride,
Valentin Cimpeanu, Georges Poncelet,
Vasile I. Parvulescu**

Journal of Molecular Catalysis A: Chemical 220
(2004) 257

Transformation of 5-hydroxymethylene-5H-6,7-dihydrodibenzo[*a,c*]cyclohepten-6-one over Ru-containing BEA zeolites

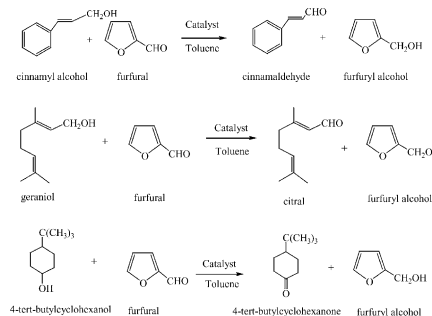


**Shu Hua Liu, Gaik Khuan Chuah,
Stephen Jaenicke**

Journal of Molecular Catalysis A: Chemical 220
(2004) 267

Liquid-phase Oppenauer oxidation of primary allylic and benzylic alcohols to corresponding aldehydes by solid zirconia catalysts

Hydrous zirconia calcined at 250–300°C and grafted zirconium 1-propoxide solid catalysts were found to be efficient for the Oppenauer oxidation of cinnamyl alcohol, geraniol and 4-*tert*-butylcyclohexanol in toluene when furfural was used as the oxidant.

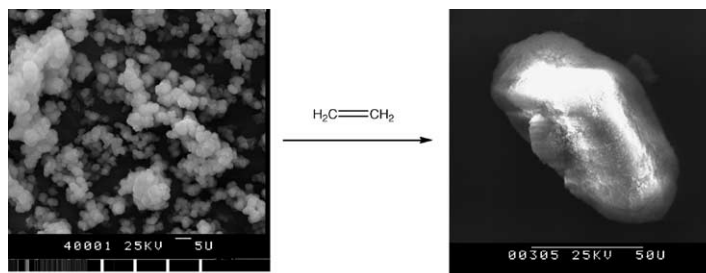


**Stefan Beck, Adrian R. Brough,
Manfred Bochmann**

Journal of Molecular Catalysis A: Chemical 220
(2004) 275

α -Zirconium phosphonates as new supports for metallocene catalysts

The chemically uniform surface structure makes zirconium phosphonates attractive as well-defined catalyst support materials. Impregnation with Cp_2ZrCl_2 by sublimation or slurry methods provide the first examples of ZrP-supported alkene polymerization catalysts, which polymerize ethene with good to excellent activities under mild conditions, even at remarkably low methylalumoxane/zirconocene ratios. The polymers form free-flowing particles which reflect the morphology of the catalyst supports.



**Carlos Alonso, Antonio Antiñolo,
Fernando Carrillo-Hermosilla,
Pedro Carrión, Antonio Otero,
José Sancho, Elena Villaseñor**

Journal of Molecular Catalysis A: Chemical 220
(2004) 285

Modified silicas as supports for single-site zirconocene catalysts

Different modified silicas have been prepared by reaction of partially dehydroxylated silica with silicon ethers [EtOSiMe₃ and (Me₃Si)₂O] or a silazane [(Me₃Si)₂NH]. The reactivity of the products towards Cp_2ZrCl_2 has been studied and compared with that of the unmodified silica. The resulting materials were activated with small amounts of MAO and the catalytic systems were evaluated in ethylene polymerization.

