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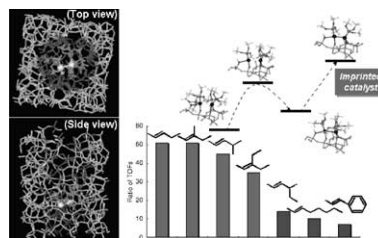
Articles

Mizuki Tada, Yasuhiro Iwasawa

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 27

Approaches to design of active structures by attaching and molecular imprinting of metal complexes on oxide surfaces

Design and catalytic performance of active metal complexes on oxide surfaces by metal-complex attaching and molecular imprinting techniques are reviewed. Metal complexes on oxide surfaces have different structures from their homogeneous analogues and often exhibit unique reactivities and catalyses. Further, metal complexes imprinted at oxide surfaces exhibit remarkable catalytic behaviors with high activity, durability, and shape selectivity.

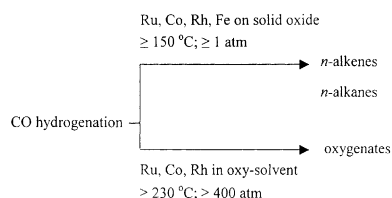


Peter M. Maitlis

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 55

Metal catalysed CO hydrogenation: hetero- or homo-, what is the difference?

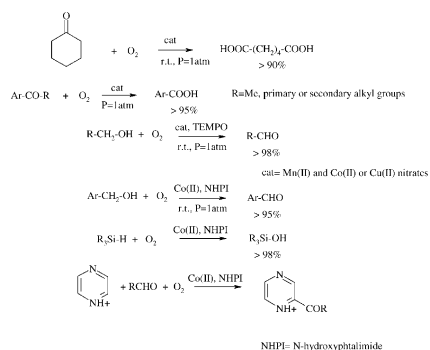
The hydrogenation of CO is *heterogeneously* catalysed by Ru, Rh, Co or Fe on silica, affording largely *n*-1-alkenes as *primary* products and working at temperatures $\geq 150^\circ\text{C}$ and pressures of syngas $\geq 1\text{atm}$. In complete contrast, the hydrogenation of CO *in solution* by Co, Rh or Ru complexes, is much more demanding and leads to oxygenates (methanol, ethanol, ethylene glycol, and formates).



Francesco Minisci, Francesco Recupero, Gian Franco Pedulli, Marco Lucarini

Journal of Molecular Catalysis A: Chemical
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Transition metal salts catalysis in the aerobic oxidation of organic compounds. Thermochemical and kinetic aspects and new synthetic developments in the presence of *N*-hydroxy-derivative catalysis

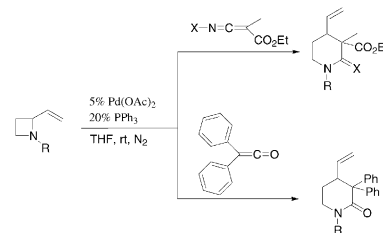


**Aina Martorell, Gyro A. Inman,
Howard Alper**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 91

Regioselective palladium-catalysed cycloaddition reactions of 1-alkyl-2-vinylazetidines with ketenimines and ketenes

1-Alkyl-2-vinylazetidines undergo regioselective cycloaddition reactions with a wide range of ketenimines and ketenes, in the presence of Pd(OAc)₂ and PPh₃ under mild conditions (room temperature and pressure), to afford six-membered ring products in moderate to good yields.

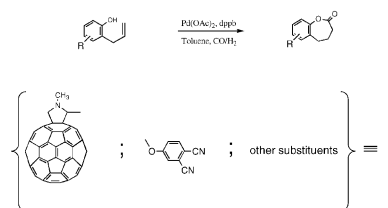


**Giuseppe Vasapollo, Giuseppe Mele,
Bassam El Ali**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 97

Catalytic and selective synthesis of lactones and bis-lactones by palladium acetate/1,4-bis(diphenylphosphino)butanesystem under syngas conditions

The combination of palladium acetate and 1,4-bis(diphenylphosphino)butane (dppb) proved once again to form an effective catalyst system for the selective cyclocarbonylation of 2-allyl phenols, bis-2-allyl phenols, steroids and other important compounds. The reactions afforded new important five-, six- and seven-membered ring lactones and bis-lactones. The seven-membered ring lactones were predominant in most reactions. This methodology can be validated for a general preparation of different substituted cyclocarbonylated and bis-cyclocarbonylated compounds.

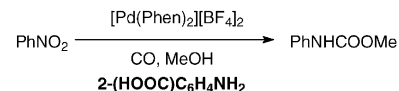


**Michela Gasperini, Fabio Ragaini,
Sergio Cenini, Emma Gallo**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 107

Carbonylation of nitrobenzene to *N*-methyl phenylcarbamate catalyzed by palladium–phenanthroline complexes. Bifunctional activation by anthranilic acid

The addition of aniline and carboxylic acids is known to promote the palladium–phenanthroline catalyzed carbonylation of nitrobenzene to methyl phenylcarbamate. Combining the amino and carboxylic functions in the same molecule and in the proper arrangement gives a further improvement in activity, but at the expense of selectivity.

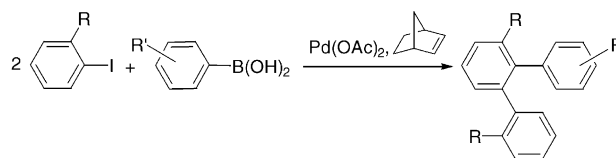


**Elena Motti, Antonella Mignozzi,
Marta Catellani**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 115

A new type of palladium-catalysed aromatic cross-coupling combined with a Suzuki reaction: synthesis of selectively 2,3'-substituted 1,1':2',1''-terphenyl derivatives

Selectively substituted terphenyl derivatives are obtained by reaction of *ortho*-substituted aryl iodides and arylboronic acids in the presence of palladium and norbornene as catalyst.

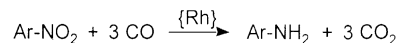


**Millan M. Mdeleleni, Robert G. Rinker,
Peter C. Ford**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 125

Reduction of aromatic nitro compounds as catalyzed by rhodium trichloride under water–gas shift reaction conditions

CO/H₂O reduction of nitroaromatics to the respective anilines under water–gas shift conditions is catalyzed by solutions prepared from RhCl₃ in aqueous amines. Effects of [CO], [Rh] and [substrate] on turnover frequencies show the nitroaromatics to be reduced by an independent catalytic cycle rather than by shift reaction produced H₂.

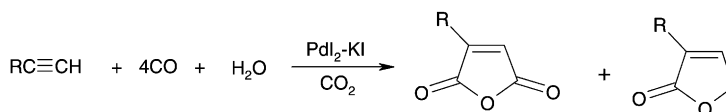


**G.P. Chiusoli, M. Costa, L. Cucchia,
B. Gabriele, G. Salerno, L. Veltri**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 133

Carbon dioxide effect on palladium-catalyzed sequential reactions with carbon monoxide, acetylenic compounds and water

While 1-alkynes with CO and H₂O in the presence of PdI₂–KI give substituted furan-2(5H)-ones deriving from a catalytic reductive carbonylation process, added CO₂ causes the formation of an equivalent amount of maleic anhydrides through a hydrogen trapping process probably involving insertion of CO₂ itself into a Pd–H bond, followed by H-transfer to form furanones.

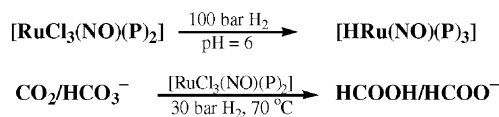


**Ágnes Kathó, Zsuzsanna Opre,
Gábor Laurency, Ferenc Joó**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 143

Water-soluble analogs of [RuCl₃(NO)-(PPh₃)₂] and their catalytic activity in the hydrogenation of carbon dioxide and bicarbonate in aqueous solution

The water-soluble complexes [RuCl₃(NO)(P)₂] were synthesized with mono- and trisulfonated triphenylphosphines, P = TPPMS or TPPTS, and characterized by IR and ¹H/³¹P NMR spectroscopies. Reactions with OH[−] yield [RuCl₃(NO₂)(P)₂]. With TPPMS/TPPTS under 100bar H₂, [RuH(NO)(P)₃] is formed which catalyze the hydrogenation of CO₂/HCO₃[−] in aqueous solutions (30bar H₂, 70°C; turnover frequencies up to 400h^{−1}).



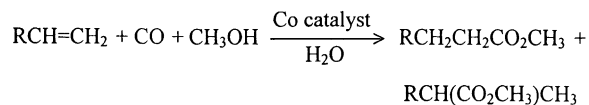
P = TPPMS, TPPTS

**Chacko Jacob, Brian T. Heaton,
Jonathan A. Iggo, Robin Whyman**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 149

Promotional effects of water and N-containing bases on Co-catalysed methoxycarbonylation of oct-1-ene

Low concentrations of water exert significant promotional effects, by factors of up to 2.5, on catalytic activity in the Co-catalysed methoxycarbonylation of oct-1-ene to esters. Although N-bases, e.g. pyridine, enhance both catalytic activity and linear product selectivity, water influences the reaction rate as strongly as pyridine.

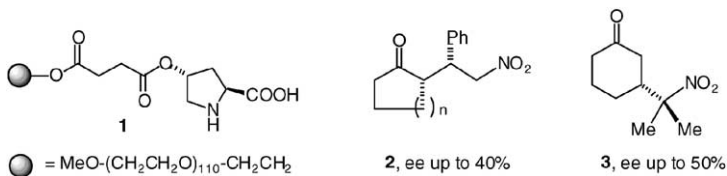


Maurizio Benaglia, Mauro Cinquini, Franco Cozzi, Alessandra Puglisi, Giuseppe Celentano

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 157

Poly(ethylene-glycol)-supported proline: a recyclable aminocatalyst for the enantioselective synthesis of γ -nitroketones by conjugate addition

A poly(ethylene-glycol)-supported proline **1** was used as the catalyst in the additions of cyclohexanone, cyclopentanone, and acetone to 2-nitrostyrene, and of 2-nitropropane to cyclohexanone. Enantiomeric excesses up to 40 and 50% were observed for products **2** and **3**, respectively. Examples of recovery and recycling of the supported catalysts in both types of processes were also reported.

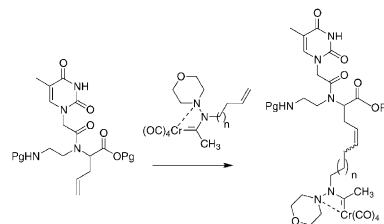


Stefano Maiorana, Emanuela Licandro, Dario Perdicchia, Clara Baldoli, Barbara Vandoni, Clelia Giannini, Michele Salmain

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 165

Synthesis of the first chiral PNA monomer labelled with a Fischer-type carbene complex

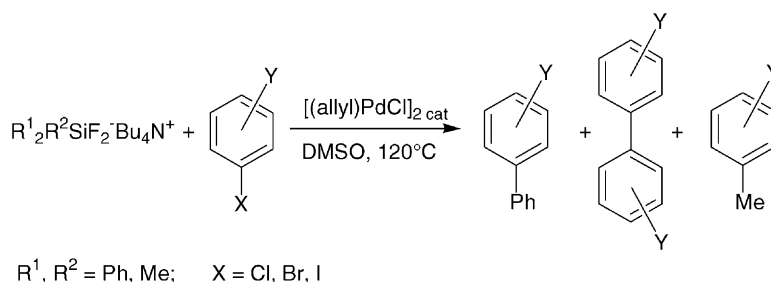
In this paper, the synthesis of the first chiral metal carbonyl labelled peptide nucleic acid (PNA) monomers is reported. IR analysis shows that the Cr(CO)₄ moiety represents a suitable spectroscopic probe for diagnostic purposes.



M. Penso, D. Albanese, D. Landini, V. Lupi

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 177

Biaryl formation: palladium catalyzed cross-coupling reactions between hypervalent silicon reagents and aryl halides

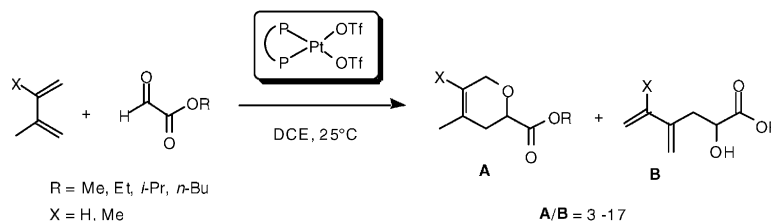


Alessandro Cendron, Giorgio Strukul

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 187

Lewis acidic platinum(II) complexes as catalysts for the hetero Diels–Alder reaction

Bis-triflate diphosphine complexes of Pt(II) can be used as catalysts for the hetero Diels–Alder reaction between simple dienes (isoprene, 2,3-dimethylbutadiene) and glyoxylate esters or simple aldehydes (benzaldehyde, terephthalaldehyde) to yield a variety of substituted dihydropyrans under mild conditions.

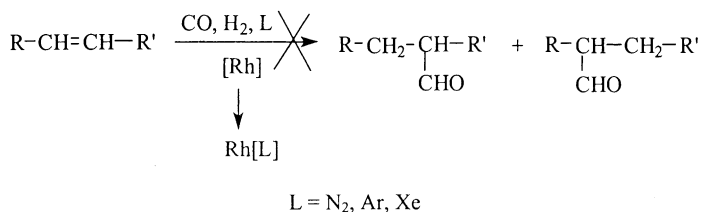


**Maria Caporali, Piero Frediani,
Franco Piacenti, Antonella Salvini**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 195

Influence of an additional gas on the rhodium-catalyzed hydroformylation of olefins

An additional gas such as dinitrogen, argon or xenon, in high concentration, reduces the initial rate of the hydroformylation of olefins (cyclohexene, hex-1-ene, styrene) catalyzed by $\text{RhH}(\text{CO})(\text{PPh}_3)_3$.

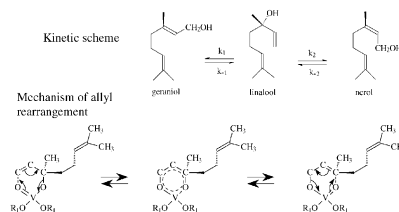


**V.A. Semikolenov, I.I. Ilyna,
R.I. Maksimovskaya**

Journal of Molecular Catalysis A: Chemical
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Linalool to geraniol/nerol isomerization catalyzed by $(\text{RO})_3\text{VO}$ complexes: studies of kinetics and mechanism

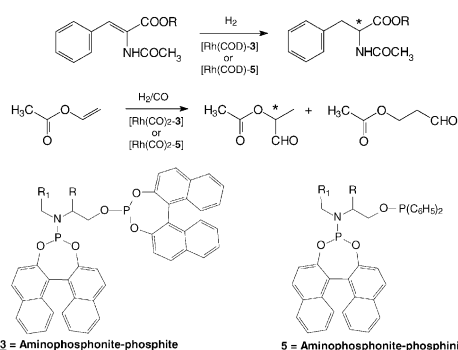
The isomerization of linalool in presence of the catalytic system $\{(\text{RO})_3\text{VO} + [(\text{Bu})_4\text{N}^+]\text{OH}\}$ is a reversible process, the equilibrium constant slightly depends on temperature and the reaction rate is of the first order on linalool, geraniol and nerol concentrations. The rate determining step of the process is the rearrangement of the coordinated to vanadium linalyl- to geranyl-(neryl-) ligands which, probably, proceeds via Red–Ox mechanism.



E. Cesarotti, S. Araneo, I. Rimoldi, S. Tassi

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 211

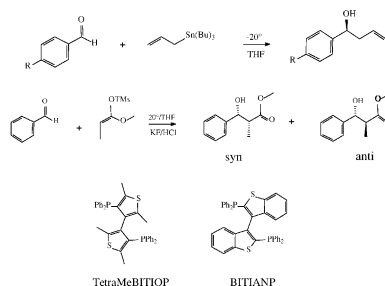
Aminophosphonite-phosphite and aminophosphonite-phosphinite ligands with mixed chirality: preparation and catalytic applications in asymmetric hydrogenation and hydroformylation



E. Cesarotti, S. Araneo, I. Rimoldi, S. Tassi

Journal of Molecular Catalysis A: Chemical
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Enantioselective Mukaiyama aldol and Sakurai allylation reactions catalysed by silver(I) complexes with chiral atropisomeric chelating ligands

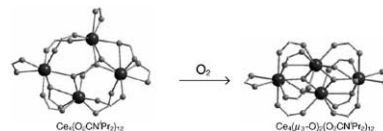


**Ulrich Baisch, Daniela Belli Dell' Amico,
Fausto Calderazzo, Luca Labella,
Fabio Marchetti, Dario Vitali**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 259

Reaction of a tetranuclear *N,N*-di-*iso*-propylcarbamato complex of cerium(III) with dioxygen: synthesis and X-ray characterization of both the oxidation product and its precursor

The tetranuclear *N,N*-di-*iso*-propylcarbamato complex of cerium(III) $Ce_4(O_2CN^iPr)_2$ and the product deriving by its oxidation with O_2 , the μ_3 -oxo tetranuclear cerium(IV) derivative $Ce_4(\mu_3-O)_2(O_2CN^iPr)_2$, have been prepared and their crystal structures solved by X-ray diffraction methods. This is the first case of a μ -oxo-carbamato complex being obtained by oxygenation, whereby product and precursor maintain the basic structural features.

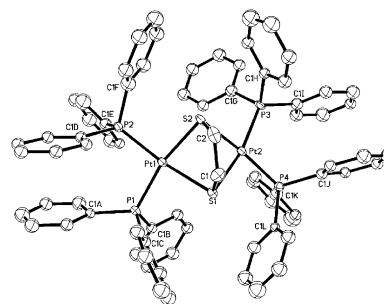


**Siew Huay Chong, Antonius Tjindrawan,
T.S. Andy Hor**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 267

Electrospray mass spectrometric investigation of the reactivity of the sulfide centers in $[Pt_2(\mu-S)_2(PPh_3)_4]$ towards organic dihalides and the catalytic potential of this complex in the syntheses of organosulfur materials

Alkylation of $[Pt_2(\mu-S)_2(PPh_3)_4]$ by 1,4-dichlorobutane, 1,2-dichloroethane, α - α' -dichloro-*o*-xylene and α - α' -dichloro-*m*-xylene has been followed by in situ electrospray mass spectroscopy (ESMS). An intermediate $[Pt_2(\mu-SC_2H_4S)(PPh_3)_4][PF_6]_2$ was isolated and characterized by single-crystal X-ray crystallographic diffractometry. The preservation of the $\{Pt_2S_2\}$ core is discussed in relation to its value in catalytic syntheses of organosulfur substrates.

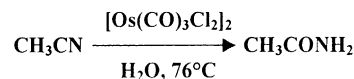


**Elena Cariati, Claudia Dragonetti,
Luca Manassero, Dominique Roberto,
Francesca Tessore, Elena Lucenti**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 279

Efficient catalytic hydration of acetonitrile to acetamide using $[Os(CO)_3Cl_2]_2$

Various osmium species are able to activate acetonitrile towards nucleophilic attack by water to give acetamide. The most efficient catalyst appears to be $[Os(CO)_3Cl_2]_2$, which gives good yields of acetamide by working in air at 76°C. The complex $[Ru(CO)_3Cl_2]_2$ is much less efficient than its osmium analogue due to its easy conversion in $[Ru(CO)_2Cl_2(CH_3CN)_2]$ under the reaction conditions.

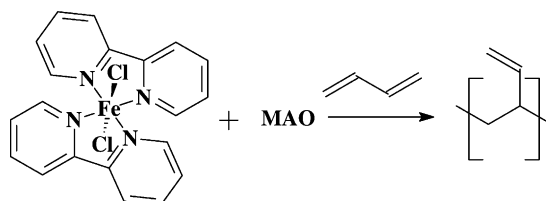


**Giovanni Ricci, Daniele Morganti,
Anna Sommazzi, Roberto Santi,
Francesco Masi**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 287

Polymerization of 1,3-dienes with iron complexes based catalysts. Influence of the ligand on catalyst activity and stereospecificity

The polymerization of 1,3-dienes with $FeCl_2 \cdot L_2/MAO$ (*L*: amine ligand) has been examined. Catalyst activity, chemo- and stereoselectivity strongly depend on the type of ligand; highly active and stereospecific catalysts are obtained in particular by using aromatic bidentate amines. These systems give 1,2-syndiotactic polybutadiene, 3,4-polyisoprene in which syndiotactic triads are predominant and *cis*-1,4-poly(2,3-dimethyl-1,3-butadiene).

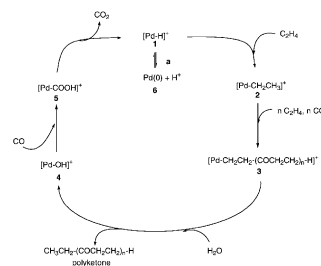


**Andrea Vavasori, Luigi Toniolo,
Gianni Cavinato, Fabiano Visentin**

Journal of Molecular Catalysis A: Chemical
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Highly active $[\text{Pd}(\text{AcO})_2(\text{dppp})]$ catalyst for the $\text{CO}-\text{C}_2\text{H}_4$ copolymerization in $\text{H}_2\text{O}-\text{CH}_3\text{COOH}$ solvent [$\text{dppp} = 1,3\text{-bis}(\text{diphenylphosphino})\text{propane}$]

The $[\text{Pd}(\text{AcO})_2(\text{dppp})]$ system in $\text{AcOH}-\text{H}_2\text{O}$ ($\text{H}_2\text{O} = 37\%$, mol/mol) yields a perfectly alternated polyketone ($27.5\text{kg/g Pd}^*\text{h}$, at 4.56MPa and 90°C) bearing only ketonic end groups. A catalytic cycle is proposed in which the insertion of C_2H_4 into $\text{Pd}-\text{H}$ bond starts the catalytic cycle and the $\text{Pd}-\text{H}$ species is reproduced through a reaction closely related to the WGS.

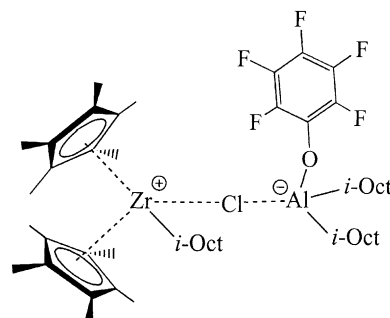


**Incoronata Tritto, Laura Boggioni,
Maria Carmela Sacchi,
Tiziano Dall'Occo**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 305

Novel aluminum based cocatalysts for metallocene catalyzed olefin polymerization

Novel cocatalysts for ethylene polymerization with metallocenes at Al/Zr molar ratios as low as 200/1 have been obtained in situ by reacting modifiers with $\text{Al}(i\text{-Bu})_3$, $\text{Al}(i\text{-Oct})_3$, and their aluminoxanes. Modifiers contain hetero-atoms and aryl groups bearing electron withdrawing substituents such as fluoro substituents or sterically encumbered groups. NMR reaction studies of $\text{C}_5\text{Me}_5\text{ZrCl}_2$ with $\text{Al}(i\text{-Oct})_3/\text{C}_6\text{F}_5\text{OH}$ demonstrate the formation of alkylated ion pair.

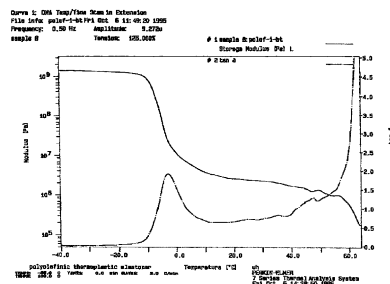


**Giuseppe Di Silvestro,
Alessandro Galbiati, Yuan Cui Ming,
Nicola Caronzolo, Edoardo Cesarotti**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 315

Polymerisation with soluble metallocene chiral catalysts: a bridge between inorganic and macromolecular stereochemistry

Criteria for an approach to the synthesis of metallocene complexes with chiral substituents and possessing proper symmetry are presented. Stereochemical results of propene polymerisation using two fluxional catalysts, different solvents and temperatures, are interpreted. Elastomeric polypropene is obtained with one catalyst. Syndiotactic polypropene was obtained with a rigid catalyst diphenylmethyl(cyclopentadienyl)(1-neomenthylindenyl)ZrCl₂.

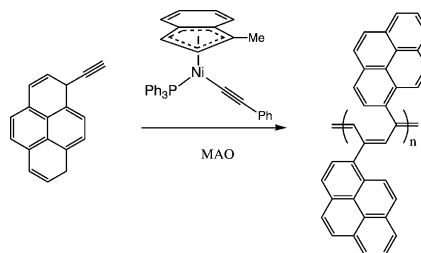


**Ernesto Rivera, Ruiping Wang,
Xiao Xia Zhu, Davit Zargarian,
Richard Giasson**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 325

Preparation of *cis*-poly(1-ethynylpyrene) using (1-Me-indenyl)(PPh_3)Ni-C≡C-Ph/methylaluminoxane as catalyst

1-Ethynylpyrene is polymerized to *cis*-poly(1-ethynylpyrene) ($M_w \sim 10^3-10^4\text{Da}$; $M_n/M_w \sim 2$) in a catalytic system composed of the complex (1-Me-indenyl)(PPh_3)Ni-C≡C-Ph and methylaluminoxane (MAO). The thermal and optical properties of these *cis*-polymers have been compared to their *trans*-analogues prepared using different catalysts.

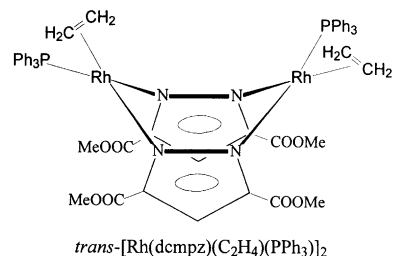


G. Attilio Ardizzoia, Stefano Brenna, Sergio Cenini, Girolamo LaMonica, Norberto Masciocchi, Angelo Maspero

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 333

Oligomerization and polymerization of alkynes catalyzed by rhodium(I) pyrazolate complexes

Three new Rh(I) derivatives containing the dcmpz ligand (Hdcmpz: 3,5-dicarbomethoxy-pyrazole) have been prepared and employed as catalysts or catalyst precursors in the cyclo-trimerization of terminal and internal alkynes and in the polymerization of ethyne to polyacetylene.

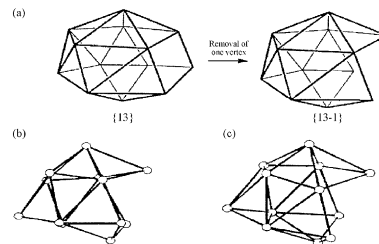


Brian F.G. Johnson, Steven Tay

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 341

The ligand polyhedral model: some further considerations of tetrahedral clusters with 12 carbonyl ligands

The three anionic clusters $[\text{Rh}_3\text{Ru}(\text{CO})_{12}]^-$, $[\text{Rh}_3\text{Os}(\text{CO})_{12}]^-$ and $[\text{Rh}_2\text{Ru}_2(\text{CO})_{12}]^{2-}$ have carbonyl polyhedral which do not readily fit within the ligand polyhedral model. It would appear that the observed polyhedra are very similar and correspond to a *nido*-capped icosahedron; as such they fall within the polyhedral growth sequence in which each successive polyhedron is generated first by edge-cleaved and then a capping operation, e.g. as with the formation of an octahedron from a trigonal bipyramid via the square-based pyramid.

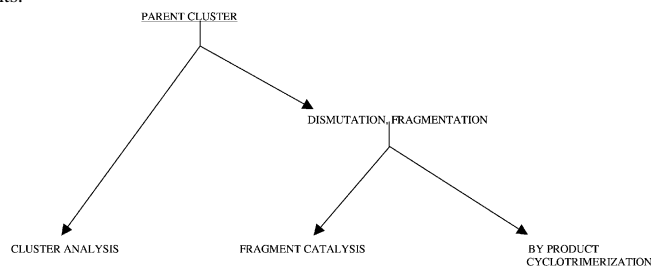


Carlo Allasia, Mario Castiglioni, Giovanni Predieri, Enrico Sappa

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 351

Reactions of diphenylacetylene and dihydrogen with chalcogenide- or methylidyne-capped trinuclear iron, ruthenium and cobalt clusters. Evidence for the formation and recombination of metal fragments

Under the conditions usually employed in the hydrogenation of diphenylacetylene, chalcogenide- and methylidyne-capped clusters undergo fragmentation and recombination of metal fragments.

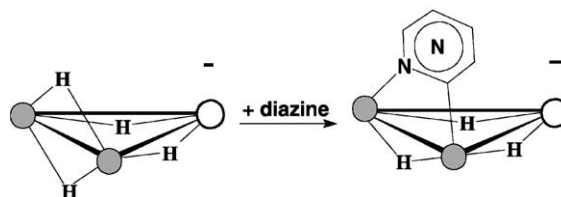


Tiziana Beringhelli, Giuseppe D'Alfonso, Daniela Maggioni, Monica Panigati, Pierluigi Mercandelli, Angelo Sironi

Journal of Molecular Catalysis A: Chemical 204–205 (2003) 361

Competition studies on the activation of the C–H bond of diazines by the unsaturated triangular cluster anion $[\text{Re}_3(\mu\text{-H})_4(\text{CO})_{10}]^-$

The activation of the *ortho* C–H bonds of 1,3- and 1,4-diazines by the unsaturated triangular cluster anion $[\text{Re}_3(\mu\text{-H})_4(\text{CO})_{10}]^-$ is slower than in the case of pyridine, but thermodynamically favoured, because orthometallated diazines are more reluctant than pyridine to undergo reductive elimination. For 1,2-diazine $\mu\text{-}\eta^2\text{-N-N}$ coordination is favoured over orthometallation.

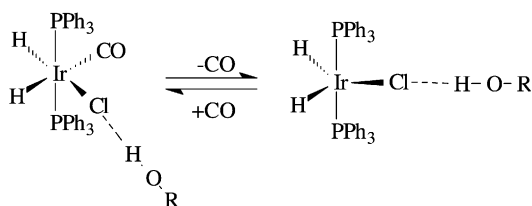


**S. Aime, A. Demaria, E. Diana,
R. Gobetto, F. Reineri**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 371

The influence of strong acidic proton donors on the reactivity of $\text{H}_2\text{Ir}(\text{CO})\text{Cl}(\text{PPh}_3)_2$ with D_2

$\text{H}_2\text{Ir}(\text{CO})\text{Cl}(\text{PPh}_3)_2$ forms intermolecular hydrogen bond with strong proton donors such as perfluorated alcohols. The formation constants of the supramolecular adducts have been evaluated and the influence of the intermolecular hydrogen bond on H_2/D_2 exchange reaction has been investigated.

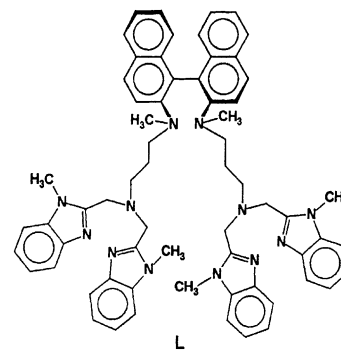


**Maria Chiara Mimmi, Michele Gullotti,
Laura Santagostini, Alberto Saladino,
Luigi Casella, Enrico Monzani,
Roberto Pagliarini**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 381

Stereoselective catalytic oxidations of biomimetic copper complexes with a chiral trinuclating ligand derived from 1,1-binaphthalene

A new polydentate ligand (L) was prepared from *R*-(+)-1,1'-binaphthyl-2,2'-diamine and was employed for the synthesis of $[\text{Cu}_2\text{L}][\text{ClO}_4]_4$ and $[\text{Cu}_3\text{L}][\text{ClO}_4]_6$. The complexes act as stereoselective catalysts in the biomimetic oxidations of the optically active catechol derivatives *L*- and *D*-Dopa and their methyl esters. In all cases, the preferred enantiomeric substrate has the *L* configuration.

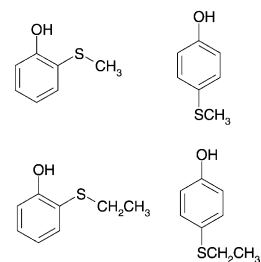


**Antonio De Riso, Michele Gullotti,
Luigi Casella, Enrico Monzani,
Antonella Profumo, Luca Gianelli,
Luca De Gioia, Noura Gaiji,
Stefano Colonna**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 391

Selectivity in the peroxidase catalyzed oxidation of phenolic sulfides

The catalytic oxidations of *ortho*- and *para*-alkylthiophenols by peroxidases exhibit various types of selectivities. Horseradish peroxidase and chloroperoxidase are active toward these substrates, although the latter enzyme addresses the oxidation preferentially on the sulfide function. Lactoperoxidase is only active with the *ortho*-substituted compounds, and the lack of reactivity toward the *para*-isomers depends on unproductive binding to the protein.

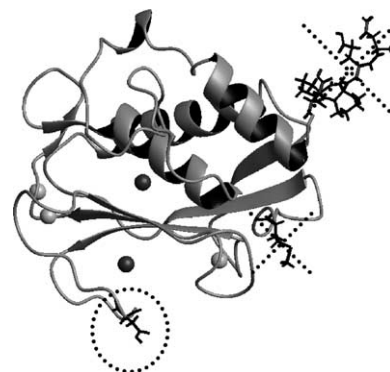


**Lucia Banci, Ivano Bertini, Alessio Ciulli,
Marco Fragai, Claudio Luchinat,
Beatrice Terzi**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 401

Expression and high yield production of the catalytic domain of matrix metalloproteinase 12 and of an active mutant with increased solubility

Single point mutations and a rational design of the construct of the catalytic domain of human metalloelastase (MMP-12) have been used to increase the solubility of the protein in order to produce optimized NMR samples for drug screening, still maintaining the full enzymatic activity.

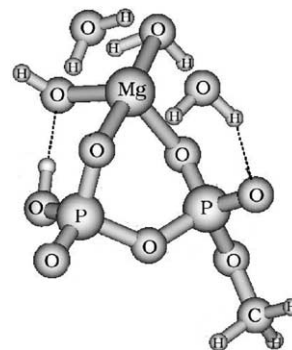


**Elena Franzini, Piercarlo Fantucci,
Luca De Gioia**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 409

Density Functional Theory investigation of guanosine triphosphate models. Catalytic role of Mg^{2+} ions in phosphate ester hydrolysis

The catalytic role of Mg^{2+} in guanosine triphosphate hydrolysis has been investigated by Density Functional Theory. The metal ion can exert its catalytic role increasing the electrophilic character of γ -phosphate (associative mechanism) or stabilizing the incipient negative charge on β -phosphate (dissociative mechanism).

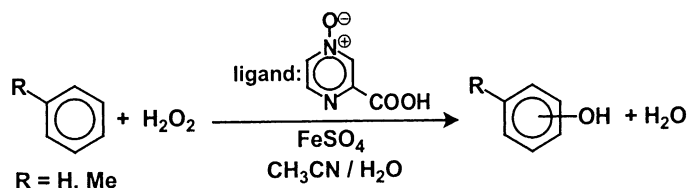


**Daniele Bianchi, Marcello Bertoli,
Roberto Tassinari, Marco Ricci,
Rodolfo Vignola**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 419

Ligand effect on the iron-catalysed biphasic oxidation of aromatic hydrocarbons by hydrogen peroxide

The effect of the ligand on the hydroxylation of benzene and toluene with hydrogen peroxide, catalysed by iron complexes in a biphasic reaction medium, was investigated. The ligand affects both the selectivity and the efficiency of the catalyst. The most effective catalyst was the complex with pyrazine-3-carboxylic acid *N*-oxide.

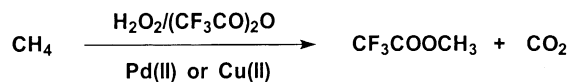


Giovanni Ingrosso, Nicola Midollini

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 425

Palladium(II)- or copper(II)-catalysed solution-phase oxyfunctionalisation of methane and other light alkanes by hydrogen peroxide in trifluoroacetic anhydride

$[Pd(hfacac)_2]$ and $[Cu(hfacac)_2(H_2O)_2]$ ($hfacac = 1,1,1,5,5,5$ -hexafluoropentane-2,4-dionate) catalyse the oxidation of methane by H_2O_2 in trifluoroacetic anhydride to the methyl trifluoroacetate, under mild conditions, CO_2 being the main by-product. Under the same conditions, ethane and propane are both more easily oxidized than methane to the corresponding trifluoroacetates.

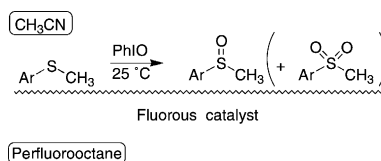


**Marco Cavazzini, Gianluca Pozzi,
Silvio Quici, Ian Shepperson**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 433

Fluorous biphasic oxidation of sulfides catalysed by (salen)manganese(III) complexes

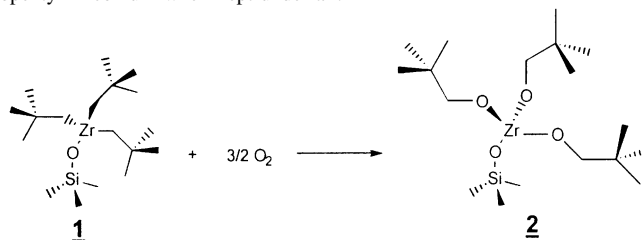
Manganese(III) complexes of heavily fluorinated salen ligands catalyze the selective oxidation of alkyl aryl sulfides with PhIO in a CH_3CN /perfluorooctane biphasic system.



**Mariko Adachi, Christophe Nédez,
Xu Xu Wang, François Bayard,
Véronique Dufaud, Frédéric Lefebvre,
Jean-Marie Basset**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 443

Surface organometallic chemistry of zirconium. Chemical reactivity of the $\equiv\text{Si}-\text{O}-\text{ZrNp}_3$ surface complex synthesized on dehydroxylated silica and application to the modification of mordenite

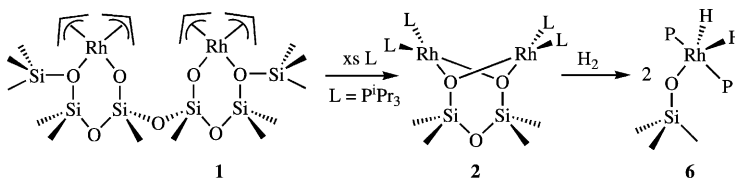


**Susannah L. Scott, Allison Mills,
Chhor Chao, Jean-Marie Basset,
Nicolas Millot, Catherine C. Santini**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 457

Silica-supported rhodium hydrides stabilized by trisopropylphosphine

A silica-supported triisopropylphosphine complex of Rh, prepared by phosphine-induced reductive elimination of allyl ligands, is proposed to be dimeric, on the basis of the ^{31}P MAS spectrum. It reacts with H_2 to give a supported Rh hydride complex and the resulting material hydrogenates butene without hydrogenolysis.

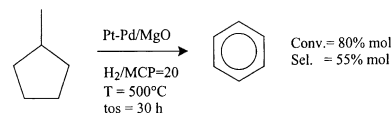


**C. Dossi, A. Pozzi, S. Recchia, A. Fusi,
R. Psaro, V. Dal Santo**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 465

An organometallic route to mono and bimetallic Pt and Pt-Pd catalysts supported on magnesium oxide: thermoanalytical investigation and catalytic behavior in MCP conversion

Bimetallic catalysts Pt-Pd/MgO prepared from organometallic complexes via solvent impregnation showed high activity and appreciable selectivity to benzene in the methylcyclopentane aromatization reaction. Their performances are comparable respect to Pt/KL systems and are superior if compared with those of monometallic Pt and Pd on MgO catalysts.

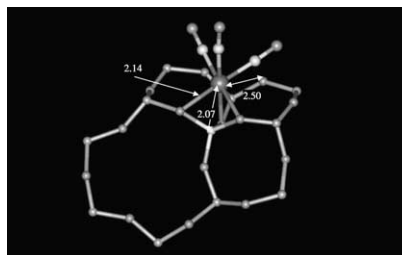


Bryan Enderle, Bruce C. Gates

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 473

Alkene hydrogenation catalyzed by rhenium carbonyls bonded to highly dealuminated Y zeolite: spectroscopic characterization of the working catalyst

Bonding of $\text{Re}(\text{CO})_3$ in zeolite DAY. Key: O, red; Si, gray; Al, light blue; C, green; Re, dark blue. Distances are given in Å. This is the precursor of a catalyst for alkene hydrogenation; changes in the coordination of the Re atom to the zeolite during catalysis were observed by EXAFS spectroscopy, and evidence of reaction intermediates was obtained by IR spectroscopy.

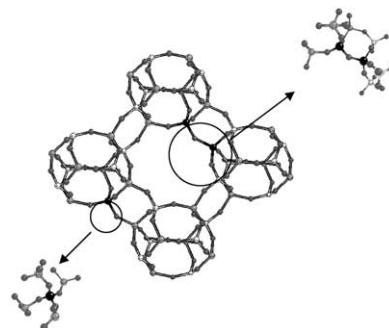


**E. Gianotti, A. Frache, S. Coluccia,
J.M. Thomas, T. Maschmeyer,
L. Marchese**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 483

The identity of titanium centres in microporous aluminophosphates compared with Ti-MCM-41 mesoporous catalyst and titanosilsesquioxane dimer molecular complex: a spectroscopy study

TAPO-34 and TAPSO-34 with chabasite-like structures were synthesised using morpholine as structure-directing agent. The synthesis and the spectroscopic characterisation (DR UV-Vis, photoluminescence and Raman spectroscopies) of these materials, combined with the study of mesoporous Ti-MCM-41 and a Titanosilsesquioxane dimer molecular complexes with a well defined co-ordination of the Ti(IV) centers, are reported.

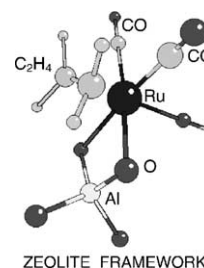


Hans Miessner

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 491

Alkene dicarbonyl complexes of Ru in a zeolite matrix. Formation and catalytic properties

Coordinatively unsaturated Ru subcarbonyls on the surface of dealuminated Y-zeolites react with olefins as ethylene and propylene in the gas phase and form well-defined olefin dicarbonyl complexes. These complexes are active and highly selective catalysts for the dimerization of ethylene.

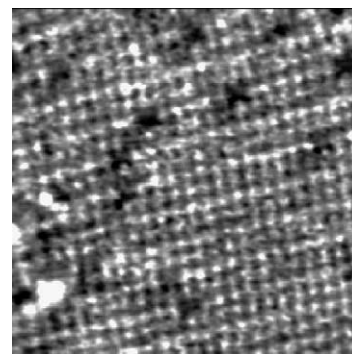


**Kevin S. Hwang, Minchul Yang,
Ji Zhu, Jeff Grunes, Gabor A. Somorjai**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 499

The molecular mechanism of the poisoning of platinum and rhodium catalyzed ethylene hydrogenation by carbon monoxide

This scanning tunneling microscope image shows the Rh(111) surface under 20mTorr H₂, 20mTorr ethylene, and 5mTorr CO. The ordered structure shown is absent until CO is introduced. From this and reaction studies, we propose a model for the CO poisoning of ethylene hydrogenation on platinum and rhodium.

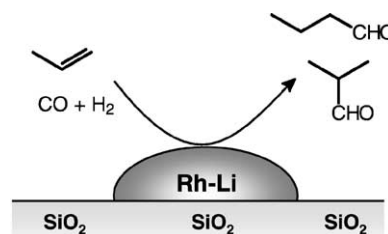


**Laura Sordelli, Matteo Guidotti,
Daniele Andreatta, Gilberto Vlaic,
Rinaldo Psaro**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 509

Characterization and catalytic performances of alkali-metal promoted Rh/SiO₂ catalysts for propene hydroformylation

The influence of alkali-metal cationic promoters on silica-supported rhodium catalysts was examined in gas-phase hydroformylation of propene at 413K. The oxidic interphase detected by Rh K-edge extended X-ray adsorption fine-structure (EXAFS) analysis is likely to be the factor responsible for the promotion effect of the catalytically active species generated by reductive carbonylation under catalytic conditions.

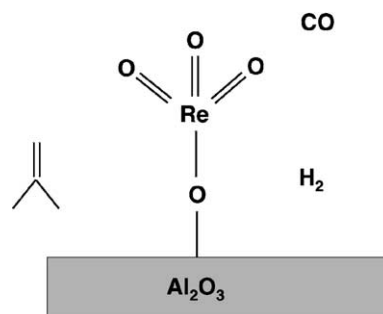


**Wayne Daniell¹, Thomas Weingand,
Helmut Knözinger**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 519

Redox properties of $\text{Re}_2\text{O}_7/\text{Al}_2\text{O}_3$ as investigated by FTIR spectroscopy of adsorbed CO

Treatment of alumina supported Re_2O_7 with H_2 at 823K leads to the complete reduction of all rhenium species to Re^0 . Partially reduced rhenium Re^{x+} (where $0 < x < 7$) species can be generated through treatment with CO or by exposure to isobutene at 333K, providing further evidence that partially reduced rhenium species are involved in the metathesis of alkenes.

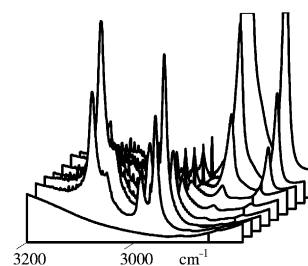


**S. Bordiga, S. Bertarione, A. Damin,
C. Prestipino, G. Spoto, C. Lamberti,
A. Zecchina**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 527

On the first stages of the ethylene polymerization on $\text{Cr}^{2+}/\text{SiO}_2$ Phillips catalyst: time and temperature resolved IR studies

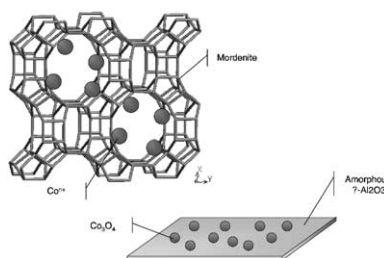
In situ, time, pressure and temperature dependent IR spectra have been collected on the $\text{Cr}^{2+}/\text{SiO}_2$ catalyst in $\text{CO}/\text{C}_2\text{H}_4$ atmosphere with the aim to identify of the species formed during the initiation of the ethylene polymerization step on the Phillips catalyst.



**E. Finocchio, T. Montanari, C. Resini,
G. Busca**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 535

Spectroscopic characterization of cobalt-containing solid catalysts

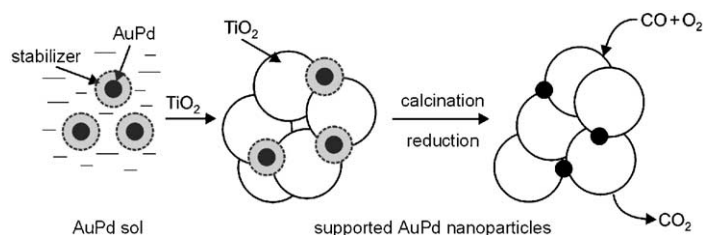


**L. Guzzi, A. Beck, A. Horváth,
Zs. Koppány, G. Stefler, K. Frey, I. Sajó,
O. Geszti, D. Bazin, J. Lynch**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 545

AuPd bimetallic nanoparticles on TiO_2 : XRD, TEM, in situ EXAFS studies and catalytic activity in CO oxidation

Tannin stabilized bimetallic AuPd nanoparticles of narrow size distribution were adsorbed on TiO_2 support from metal sol. The catalytic activity of the calcined/reduced AuPd/ TiO_2 in CO oxidation revealed a slight synergistic effect compared to the activity of monometallic analogous referred to the Au and Pd surface area in the bimetallic sample.

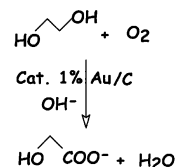


Francesca Porta, Michele Rossi

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 553

Gold nanostructured materials for the selective liquid phase catalytic oxidation

Au(0) sols were obtained by reduction of aqueous solution of NaAuCl₄ with NaBH₄, in the presence of protective agents (polymers and surfactants). The sols consisted of nanoparticles of different size (2.6–6.9 nm by TEM) on depending of the stabilizer. They were immobilized on activated carbon and the heterogeneous catalysts tested in a model reaction for the selective liquid phase oxidation of ethylene glycol to glycolate. A comparison of the catalytic activities underlines the importance of the stabilizer in both the steps of sol formation and support impregnation.

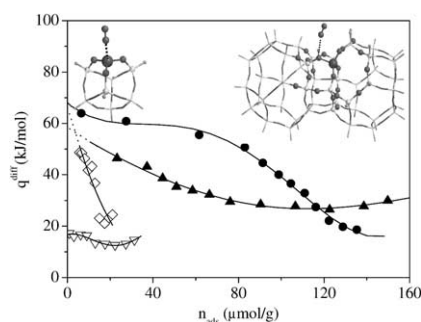


Glycol / Au = 1000
Glycol / NaOH = 0.5
t = 1 h
pO₂ = 300 kPa
T = 343 K

V. Bolis, M. Broyer, A. Barbaglia, C. Busco, G.M. Foddanu, P. Ugliengo

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 561

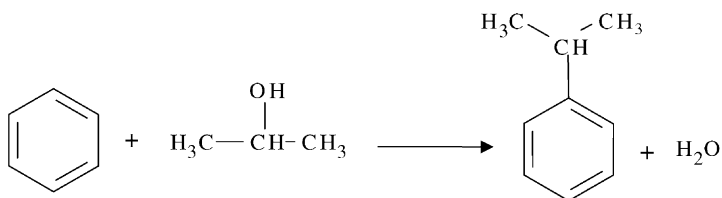
Van der Waals interactions on acidic centres localized in zeolites nanocavities: a calorimetric and computer modeling study

**Gianni Girotti, Franco Rivetti, Stefano Ramello, Lino Carnelli**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 571

Alkylation of benzene with isopropanol on β-zeolite: influence of physical state and water concentration on catalyst performances

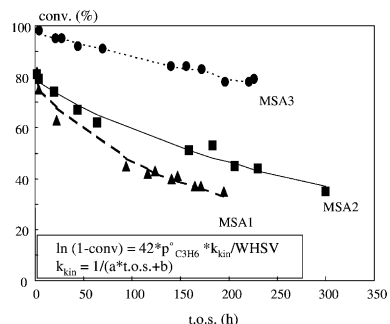
In β-zeolite catalyzed direct alkylation of benzene to cumene by isopropanol performances comparable to the current industrial propylene-based process have been obtained, overcoming the expected drawbacks due to the presence of a large quantity of stoichiometrical water in the reaction mixture. These results have paved the road toward a viable acetone recycle in phenol production.

**C. Flego, S. Peratello, C. Perego, L.M.F. Sabatino, G. Bellussi, U. Romano**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 581

Reaction and deactivation study of mesoporous silica–alumina (MSA) in propene oligomerisation

Deactivation of mesoporous silica–alumina (MSA) is investigated in propene oligomerisation. The initial activity is correlated with the Lewis acid sites. Part of them is poisoned at the beginning of the reaction, the decay rate being consistent with their strength. At longer reaction time pore blockage, caused by an increased dimension of the adsorbed organic residues, becomes the main side phenomenon.

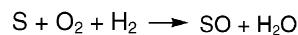


**N.I. Kuznetsova, N.V. Kirillova,
L.I. Kuznetsova, V.A. Likholobov**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 591

Oxidation of hydrocarbons by dioxygen reductively activated on platinum and heteropoly compounds

Based on Pt and heteropoly compounds (HPC), catalysts are applied to oxygenation of hydrocarbon substrates S (S = cyclohexane, cyclohexene, and α -pinene) in liquid phase with a mixture of O₂ and H₂ gases. Activity of the catalytic systems and composition of the oxygenated products are controlled by the nature of active intermediates generated under the action of the different HPC.

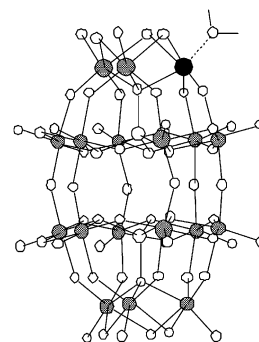


**Fabrizio Cavani, Roberto Mezzogori,
Alessandro Trovarelli**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 599

The characterization and the catalytic activity of modified Wells–Dawson-type polyoxometalates in the oxidativehydrogenation of isobutane to isobutene

Wells–Dawson heteropolycompounds of the type K₁₀P₂W₁₇O₆₁ and the metal-substituted K₇P₂W₁₇MO₆₁ are active and selective in isobutane oxidativehydrogenation to isobutene. A high activity is evident only under conditions which favour the polyoxometallate reduction, and the likely generation of radical species which propagate in the gas phase, thus yielding a reactivity typical of heterogeneously-initiated, homogeneous reactions.



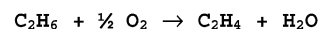
L. Lisi, P. Patrono, G. Ruoppolo

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 609

Vanadyl phosphate dihydrate supported on oxides for the catalytic conversion of ethane to ethylene

Bulk and supported VOPO₄ were investigated for oxidative dehydrogenation of ethane at 450–550°C. The improvement of catalytic activity for supported catalysts was related to the increase of both surface area and reducibility enhanced in extent depending on the strength of the interaction with support. Ethylene selectivity increases with temperature for better dispersed samples due to an increase of V(IV) at 550°C.

**Oxidative
Dehydrogenation**

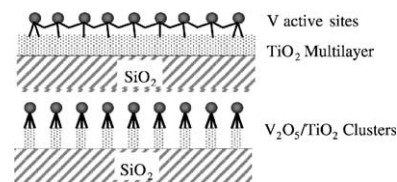


**E. Santacesaria, A. Sorrentino, R. Tesser,
M. Di Serio, A. Ruggiero**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 617

Oxidative dehydrogenation of ethanol to acetaldehyde on V₂O₅/TiO₂-SiO₂ catalysts obtained by grafting vanadium and titanium alkoxides on silica

Oxidative dehydrogenation of ethanol to acetaldehyde has been studied on catalysts prepared by grafting vanadyl tri-isopropoxide on silica coated with TiO₂ or alternatively by reacting vanadyl tri-isopropoxide with titanium tetra-isopropoxide and grafting the obtained bimetallic alkoxide directly on silica. This catalyst resulted less active but more selective in the mentioned reaction. The difference between the mentioned catalysts is depicted in the scheme showing more V–O–Ti instead of V–O–V bonds for the selective catalyst.

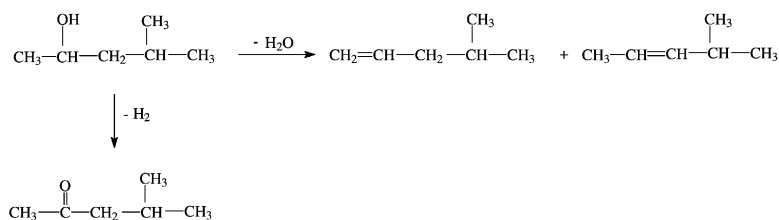


**V. Solinas, E. Rombi, I. Ferino,
M.G. Cutrufello, G. Colón, J.A. Navío**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 629

Preparation, characterisation and activity of
CeO₂-ZrO₂ catalysts for alcohol dehydration

Ceria-zirconia catalysts have been prepared in a wide range of composition and characterised as to their structure, texture, surface composition and acid–base features. Their activity for the conversion of 4-methylpentan-2-ol has been tested. The competition among the reaction pathways sketched below is governed by the concentration and strength of the acid and basic sites.

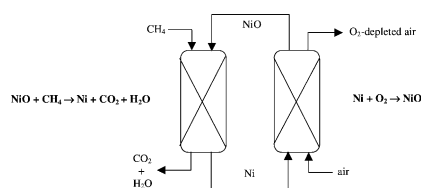


**Raffaella Villa, Cinzia Cristiani,
Gianpiero Groppi, Luca Lietti,
Pio Forzatti, Ugo Cornaro,
Stefano Rossini**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 637

Ni based mixed oxide materials for CH₄
oxidation under redox cycle conditions

The preparation, characterization and redox properties of Ni–Al–O (Ni/Al = 0.5–2.25) and Ni–Mg–Al–O mixed oxides (synthesized via coprecipitation) for CH₄ chemical looping combustion (CLC) is investigated. Temperature programmed reduction with H₂ (H₂-TPR) and temperature programmed reduction with CH₄ (CH₄-TPR) tests—followed by temperature programmed oxidation (TPO) runs—are performed on the catalysts, along with CH₄/O₂ pulse experiments in the presence and in the absence of water.

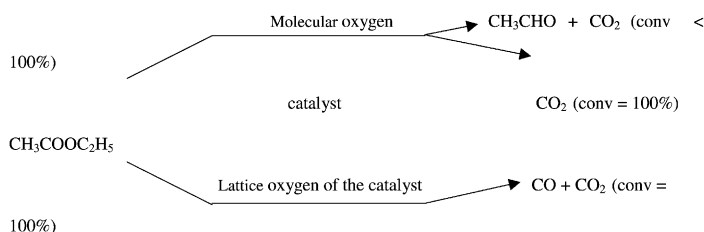


C. Mazzocchia, A. Kaddouri

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 647

On the activity of copper chromite catalysts
in ethyl acetate combustion in the presence
and absence of oxygen

The catalytic combustion of ethyl acetate was studied over a series of undoped and doped copper chromite catalysts. The role of the promoters and the red–ox process of the Mn/CuO–CuCr₂O₄ system have been evidenced by tests carried out in the absence and in the presence of oxygen. The results are interpreted in terms of both lattice oxygen and Cu²⁺/Cu⁺ ratio.

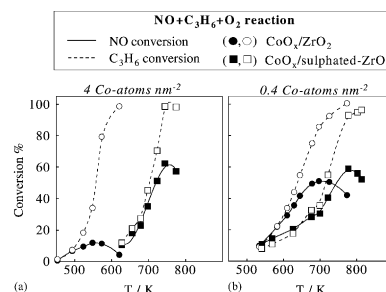


**Valerio Indovina, Daniela Pietrogiacomi,
Maria Cristina Campa**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 655

The catalytic activity of CoO_x/sulphated-
ZrO₂ for the NO abatement with C₃H₆ in
the presence of O₂: the dependence of activity
and selectivity on the sulphate content

CoO_x/sulphated-ZrO₂ containing 4 Co-atoms
nm⁻² were far more active and selective than
the corresponding unsulphated CoO_x/ZrO₂
(section a). The presence of sulphates had a
weaker effect on samples with 0.4 Co-atoms
nm⁻² (section b). Cobalt and sulphate coop-
erate in determining the activity and selec-
tivity of CoO_x/sulphated-ZrO₂ catalysts.

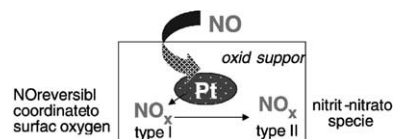


Gabriele Centi, Giuseppe E. Arena

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 663

NO reduction by C_3H_6 and O_2 over supported noble metals. Part I. Role of the support on the nature of NO_x adspecies and their relationship with the catalytic behaviour

NO thermodesorption studies and in situ DRIFT experiments on Pt supported on alumina, titania and titania–alumina indicate a relationship between activity in NO reduction by propene/ O_2 and amount of weakly coordinated NO species (type I) and their rate of transformation to stronger chemisorbed NO_x species (type II).

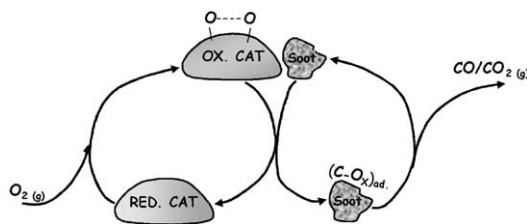


P. Ciambelli, V. Palma, P. Russo, S. Vaccaro

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 673

Redox properties of a TiO_2 supported Cu-V-K-Cl catalyst in low temperature soot oxidation

In this work we propose that the Cu-V-K-Cl based catalyst is active towards the soot oxidation through a redox mechanism: (i) the catalyst is reduced by soot; (ii) $(C-O)_x$ complexes are formed on soot surface; (iii) CO and CO_2 are produced; (iv) the reduced catalyst is re-oxidised by gaseous oxygen.

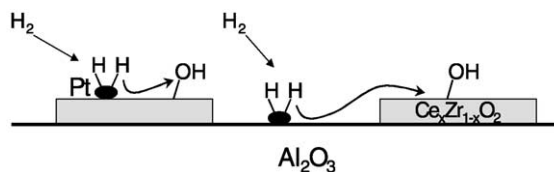


P. Fornasiero, J. Kaspar, T. Montini, M. Graziani, V. Dal Santo, R. Psaro, S. Recchia

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 683

Interaction of molecular hydrogen with three-way catalyst model of $Pt/Ce_{0.6}Zr_{0.4}O_2/Al_2O_3$ type

Efficient H_2 activation and spillover is observed on Pt/CeO_2-ZrO_2 even after supporting the system on Al_2O_3 .

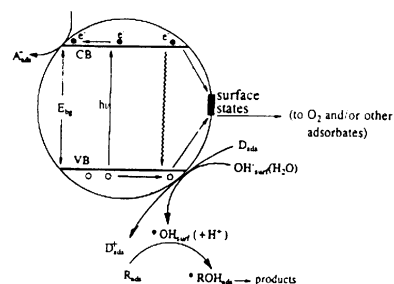


P. Davit, G. Martra, S. Coluccia, V. Augugliaro, E. García López, V. Loddo, G. Marci, L. Palmisano, M. Schiavello

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 693

Adsorption and photocatalytic degradation of acetonitrile: FT-IR investigation

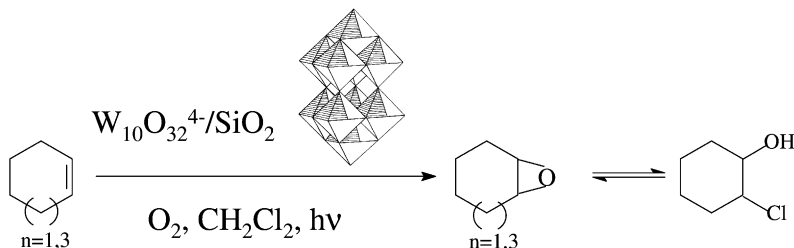
Acetonitrile photodegradation was performed in aqueous suspensions of TiO_2 Degussa P25 and TiO_2 Merck; the latter photocatalyst exhibited an initial higher conversion rate. FT-IR investigations showed that acetonitrile adsorption is reversible only for TiO_2 Merck. Photostable acetamide-like species formed on TiO_2 P25 could poison some photocatalytic sites, accounting for the lower initial conversion rate.



**A. Maldotti, R. Amadelli, I. Vitali,
L. Borgatti, A. Molinari**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 703

CH₂Cl₂-assisted functionalization of cycloalkenes by photoexcited (nBu₄N)₄W₁₀O₃₂ heterogenized on SiO₂

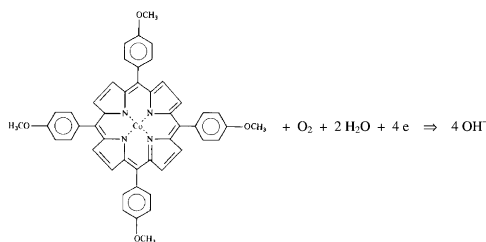


Cristina Mocchi, Sergio Trasatti

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 713

Composite electrocatalysts for molecular O₂ reduction in electrochemical power sources

Composite electrocatalysts for molecular O₂ reduction with higher activity than pyrolyzed cobalt tetramethoxy-phenylporphyrin (CoTMPP) were synthesized by pyrolyzing a mixture of CoCO₃ + TMPP + carbon black in an inert atmosphere. Maximum activation was observed at 800°C.

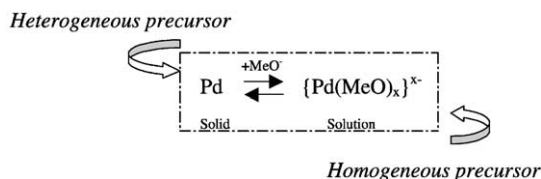


**Carlo Carlini, Marco Di Girolamo,
Alessandro Macinai, Mario Marchionna,
Marilena Noviello,
Anna Maria Raspolli Galletti,
Glaucio Sbrana**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 721

Synthesis of isobutanol by the Guerbet condensation of methanol with *n*-propanol, has been studied. Bifunctional catalysts based on either heterogeneous or homogeneous dehydrogenating/hydrogenating palladium species and on sodium methoxide as basic component were investigated. It was observed that both homogeneous or colloidal and heterogeneous palladium species contributed to the overall activity; they are likely in equilibrium according to the following scheme:

The catalytic synthesis of isobutanol via the Guerbet condensation of methanol with *n*-propanol, has been studied. Bifunctional catalysts based on either heterogeneous or homogeneous dehydrogenating/hydrogenating palladium species and on sodium methoxide as basic component were investigated. It was observed that both homogeneous or colloidal and heterogeneous palladium species contributed to the overall activity; they are likely in equilibrium according to the following scheme:

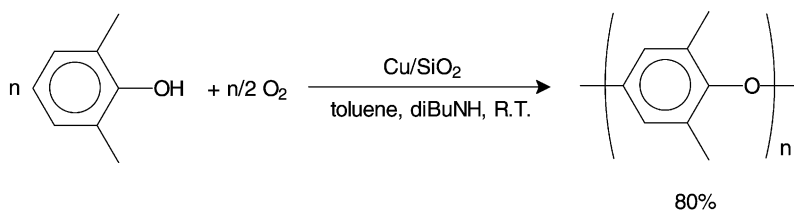


**Mauro Ercoli, Achille Fusi, Rinaldo Psaro,
Nicoletta Ravasio, Federica Zaccheria**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 729

Cu/SiO₂: a step forward in the heterogenization of the 2,6-dimethyl-phenol polymerization catalytic system

The polymerization of 2,6-dimethyl-phenol to polyphenylene-ether can be carried out over a 8% Cu/SiO₂ catalyst in toluene/dibutylamine. The metal leaching under these conditions is reduced to <3% and the reaction is shown to be truly heterogeneous.

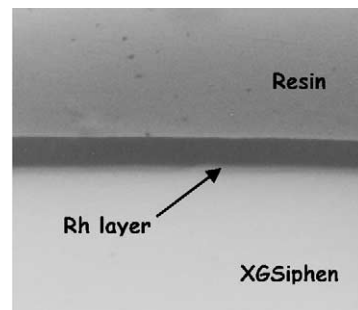


**Lisa Balzano, Daniele Cauzzi,
Diego Cauzzi, Claudio Mucchino,
Giovanni Predieri, Antonio Tiripicchio**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 737

Leaching of anchored Rh and Pd species from thiourea-functionalized monolithic silica xerogel catalyzes

Thiourea-functionalized hybrid monoliths were prepared by sol–gel method. Rh(I) and Pd(II) species were anchored through sulphur co-ordination on the surface of the monoliths obtained from 1,4-[(EtO)₃Si(CH₂)₃NHC(S)NH]₂(C₆H₄) (XGSiphen). Rh(I) anchored metal complexes were spectroscopically identified by FTIR microspectrometry. The metal leaching was determined, using plasma atomic emission spectrometry, in the hydroformylation (Rh) and hydrogenation (Pd) of styrene.

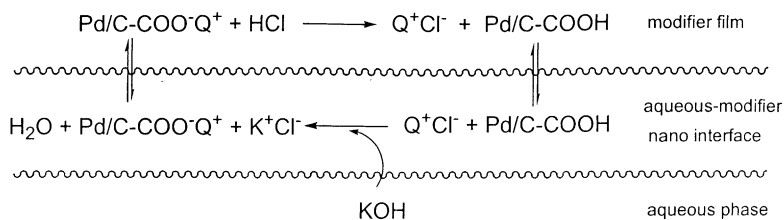


**Pietro Tundo, Alvise Perosa,
Sergei Zinovyev**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 747

Modifier effects on Pt/C, Pd/C, and Raney-Ni catalysts in multiphase catalytic hydrogenation systems

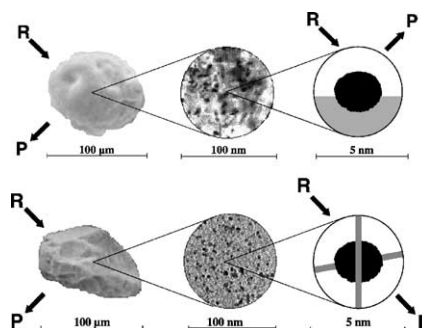
The presence of a modifier, e.g. an ammonium salt, in the isooctane–aqueous medium promotes rates increases and interesting regio-, chemo-, or enantioselectivities in multiphase catalytic reduction reactions. The modifier forms nanoenvironment on the catalyst surface, wherein the reaction proceeds.



B. Corain, P. Centomo, S. Lora, M. Kralik

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 755

Functional resins as innovative supports for catalytically active metal nanoclusters

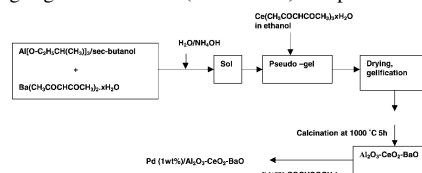


L.F. Liotta, G. Deganello

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 763

Thermal stability, structural properties and catalytic activity of Pd catalysts supported on Al₂O₃–CeO₂–BaO mixed oxides prepared by sol–gel method

Al₂O₃–CeO₂–BaO mixed oxides were prepared by sol–gel method and the influence of barium and cerium on the thermal stability of both supports and palladium catalysts was investigated by X-ray diffraction (XRD), BET surface area and pore size distribution measurements. It was found that the addition of barium improves the thermal stability of alumina and favors the ceria crystallites dispersion. Activity tests in methane combustion performed on the Pd–AlCeBa_x series show that low-ceria loaded (4–8wt.%) catalysts exhibit better light-off performances than the corresponding high-ceria loaded (12–16wt.%) samples.

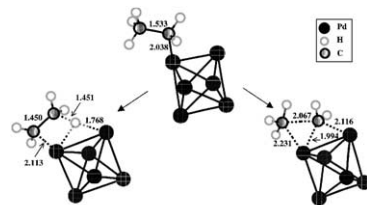


**Valeria Bertani, Carlo Cavallotti,
Maurizio Masi, Sergio Carrà**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 771

A theoretical analysis of the molecular events involved in hydrocarbons reactivity on palladium clusters

The reactivity of small hydrocarbons over palladium clusters, containing up to seven atoms, was investigated through density functional theory. The interaction of the clusters with hydrogen, methane, ethane and their fragments was investigated and the kinetic constants of the most important reactions were calculated with transition state theory. On the basis of these results a simple kinetic scheme was developed.



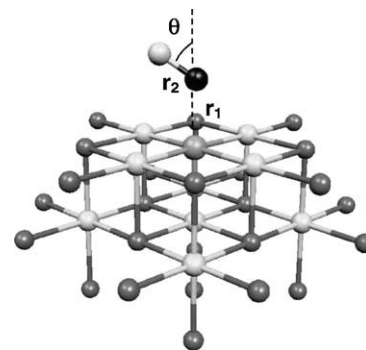
Calculated structure of transition states for the two channels-decomposition of C_2H_2 adsorbed over a Pd_4 cluster

**Mario Chiesa, Maria Cristina Paganini,
Elio Giamello, Cristiana Di Valentin,
Gianfranco Pacchioni**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 779

Bonding of NO on $Ni_xMg_{1-x}O$ powders: an EPR and computational study

The reactivity of the paramagnetic NO molecule with Ni-doped MgO is studied by electron paramagnetic resonance and density functional theory. We observe the formation of two species, NO physisorbed on low-coordinated Mg^{2+} ions and NO adsorbed on terrace Ni^{2+} ions. The NO– Ni^{2+} bonding is relatively strong with dominant covalent character, and is characterized by the presence of one unpaired electron localized on the Ni 3d shell, which formally assumes a $3d^9$ configuration.

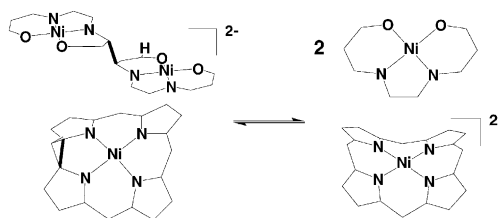


**Paola Belanzoni, Simona Fantacci,
Marzio Rosi, Antonio Sgamellotti**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 787

A theoretical approach to a chemical system convertible into a storage cell: carbon–carbon bonds functioning as electron donor and electron acceptor units

Density functional calculations have been performed on nickel Schiff base complexes and nickel porphyrinogen complexes in order to understand the behaviour of these systems in redox processes. Their complementary behaviour in redox processes can be considered in a reversible electrochemical cell with the discharge process based on C–C bonds breaking and the recharge based on C–C bonds formation.



**Maurizio Bruschi, Piercarlo Fantucci,
Maddalena Pizzotti, Cristina Rovizzi**

Journal of Molecular Catalysis A: Chemical
204–205 (2003) 793

Tailoring transition metal complexes for non linear optics applications. A theoretical investigation of the electronic structure of $M(CO)_xCl_yL$ complexes ($M = Cr, W, Re, Ru, Os, Rh, Ir$; $L = Pyz, PyzBF_3, BPE, BPBEF_3$)

A density functional theory (DFT) investigation of molecular and electronic structure of $M(CO)_xCl_yL$ complexes ($M = Cr, W, Re, Ru, Os, Rh, Ir$; $L = Pyz, PyzBF_3, BPE, BPBEF_3$) shows that the magnitude and the orientation of the dipole moment are strongly affected by the presence of BF_3 group and Cl^- ligands. Influence of such features on non linear optical (NLO) properties are also discussed.

