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# **Articles**

#### W. Keim

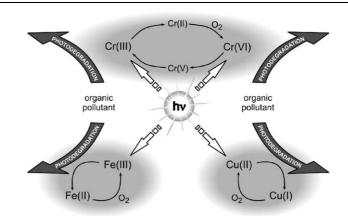
Journal of Molecular Catalysis A: Chemical 224 (2004) 11

Coordination geometry and bio-inspired ligands: useful concepts in homogeneous catalysis? A conceptual view

# Paweł Cieśla, Przemysław Kocot, Piotr Mytych, Zofia Stasicka

Journal of Molecular Catalysis A: Chemical 224 (2004) 17

Homogeneous photocatalysis by transition metal complexes in the environment



Claudio Bianchini, Andrea Meli, Werner Oberhauser, Sebastien Parisel, Oleg V. Gusev, Alexander M. Kal'sin, Nikolai V. Vologdin, Fedor M. Dolgushin

Journal of Molecular Catalysis A: Chemical 224 (2004) 35

Methoxycarbonylation of styrene to methyl arylpropanoates catalyzed by palladium(II) precursors with 1,1'-bis(diphenylphosphino)metallocenes

The selective methoxycarbonylation of styrene to methyl phenylpropanoates, with large prevalence of the linear regioisomer, can be achieved by 1,1'-bis(diphenylphosphino)metallocenyl palladium(II) catalysts. The presence of methyl substituents on the cyclopentadienyl ligands, and the type of metal in the metallocenyl unit, which may vary from iron to ruthenium to osmium, control the catalytic activity.

# Lori A. Watson, Maren Pink, Kenneth G. Caulton

Journal of Molecular Catalysis A: Chemical 224 (2004) 51

The fate of nitric oxide in its reaction with the 14-valence-electron planar species [('Bu<sub>2</sub>PCH<sub>2</sub> SiMe<sub>2</sub>)<sub>2</sub>N]RuCl

The 14 valence electron, "doubly unsaturated" (PNP)RuCl consumes multiple NO molecules, with oxygen transfer, to produce NO<sub>2</sub><sup>-</sup> ligands.

 $P^NP = (^tBu_2PCH_2SiMe_2)_2N$ 

Sandra Bolaño, Luca Gonsalvi, Fabrizio Zanobini, Francesco Vizza, Valerio Bertolasi, Antonio Romerosa, Maurizio Peruzzini

Journal of Molecular Catalysis A: Chemical 224 (2004) 61

Water soluble ruthenium cyclopentadienyl and aminocyclopentadienyl PTA complexes as catalysts for selective hydrogenation of  $\alpha,\beta$ -unsaturated substrates (PTA=1,3,5-triaza-7-phosphaadamantane)

$$Cp(CH_2)_2NEt_2 + KO^tBu \xrightarrow{trans-[RuCl_2(PPh_3)_3]} Cl \xrightarrow{Ru}_{PPh_3} NEt_2$$

$$Cl \xrightarrow{Ru}_{PPh_3} PPh_3 \qquad \textbf{(3)}$$

$$Cl \xrightarrow{Ru}_{PPh_3} PPh_3 \qquad \textbf{(3)}$$

$$Cl \xrightarrow{Ru}_{PTA} PTA \qquad \textbf{(4)} \qquad toluene reflux$$

Maria B. Ezhova, Brian O. Patrick, Brian R. James, Francis J. Waller, Michael E. Ford

Journal of Molecular Catalysis A: Chemical 224 (2004) 71

New chiral *N*,*P*-oxazolines, and their Ir complexes in asymmetric hydrogenation of an imine

# W. Wojtków, A.M. Trzeciak, R. Choukroun, J.L. Pellegatta

Journal of Molecular Catalysis A: Chemical 224 (2004) 81

Pd colloid-catalyzed methoxycarbonylation of iodobenzene in ionic liquids

A Pd colloid prepared by reduction of the  $[Pd(\eta^3-allyl)_2Cl]_2$  precursor with  $Vcp_2$  (vanadocene) in the presence of polyvinylpyrrolidone (PVP) as a protecting polymer was found to be an active and stable catalyst of methoxycarbonylation of iodobenzene carried out in an ionic liquid (IL) medium. At the optimal reaction conditions, the yield of methoxycarbonylation catalyzed by Pd colloid decreases in the order:  $[^nBu_4N]Br > [^nBu_4N]I > [^nBu_4N]Cl > [bumepy]PF_6 > [Et_4N]Br > [bumepy]Cl > [bumepy]BF_4 > [Et_4N]Cl > [bmim]PF_6 > [bmim]BF_4 > [bmim]Cl.$ 

#### István Jószai, Ferenc Joó

Journal of Molecular Catalysis A: Chemical 224 (2004) 87

Hydrogenation of aqueous mixtures of calcium carbonate and carbon dioxide using a water-soluble rhodium(I)-tertiary phosphine complex catalyst

A mild method has been developed for the hydrogenation of calcium carbonate to calcium formate in aqueous suspensions under  $CO_2 + H_2$  pressure catalyzed by [RhCl(mtppms)<sub>3</sub>] (mtppms = monosulfonated triphenylphosphine) at  $20-70~^{\circ}C$  and 10-100 bar total pressure. In certain cases the yield of formate exceeded 100% (based on CaCO<sub>3</sub>) which implies the concomitant hydrogenation of carbon dioxide, too.

CaCO<sub>3</sub> 
$$\xrightarrow{H_2 + \text{CO}_2\text{H} + 2\text{O}}$$
  $\text{Ca}(\text{HCO}_2)_2$   $\text{Ca}(\text{HCO}_2)_2$   $\text{P}(\text{H}_2) = 2\text{-80 bar}$   $\text{Ptppms} = \text{Ph}_2\text{P}$   $\text{SO}_3\text{Na}$   $\text{T} = 20\text{-}70 \,^{\circ}\text{C}$ 

# Jolanta Ejfler, Michał Kobyłka, Marek Hojniak, Piotr Sobota

Journal of Molecular Catalysis A: Chemical 224 (2004) 93

The influence of cocatalysts on phenylacetylene oligo- and polymerization

Catalytic properties of titanium bisphenolate complexes with 2,2'-ethylidenebis-(4,6-di-*tert*-butylphenol) (edbpH<sub>2</sub>) towards polymerization of phenylacetylene (PA) are reported. It was found that the catalytic activity and products formation depend strongly on the used cocatalyst AlR<sub>3</sub> (R = Me, Et,  $^{i}$ Bu). *trans*-PPA was formed when [Ti(edbp)Cl<sub>2</sub>]/AlEt<sub>3</sub> catalytic system was explored and cyclotrimerization products for [Ti(edbp)Cl<sub>2</sub>]/Al $^{i}$ Bu<sub>3</sub> catalyst.

Robert Skeřil, Pavel Šindelář, Zdenek Salajka, Vojtech Varga, Ivana Císařová, Jiří Pinkas, Michal Horáček, Karel Mach

Journal of Molecular Catalysis A: Chemical 224 (2004) 97

Copolymerization of ethene with styrene using CGC catalysts: the effect of the cyclopentadienyl ligand substitution on the catalyst activity and copolymer structure

Catalysts 1/MAO–3/MAO at molar ratios Al/Ti = 900 and styrene/ethene = 10 at 50  $^{\circ}$ C produced pseudo-random copolymer containing up to 47.8 mol% of incorporated styrene.

# Angela Sorkau, Kerstin Schwarzer, Christoph Wagner, Eike Poetsch, Dirk Steinborn

Journal of Molecular Catalysis A: Chemical 224 (2004) 105

Dimerization and cyclotrimerization of aldehydes: ruthenium catalyzed formation of esters, 1,3,5-trioxanes, and aldol condensation products from aldehydes

 $[RuCl(SiMe_3)(CO)(PPh_3)_2] \ was \ found to \ catalyze \ dimerization \ of \ aldehydes \ RC(O)H \ yielding \ esters \ RC(O)-OCH_2R \ in \ a \ Tishchenko \ type \ reaction. \ [RuCl(H)(CO)(PPh_3)_3] \ did \ not \ act \ as \ catalyst \ yielding \ esters, but in the presence of \ H_2C = CHSiMe_3 \ catalytic \ formation \ of \ cyclotrimers \ of \ aldehydes \ (RCHO)_3 \ and \ aldol \ condensation \ products \ RCH = CR'-C(O)H \ was \ observed.$ 

# Bogdan Marciniec, Dariusz Chadyniak, Stanisław Krompiec

Journal of Molecular Catalysis A: Chemical 224 (2004) 111

Ruthenium catalyzed cross-metathesis versus silylative coupling of vinyl and allyl sulfides with vinylsilanes A new catalytic route for synthesis of unsaturated organosilicon compounds with vinylic functionality  $(R'O)_3SiCH=CH(CH_2)_nSR$  (where R=t-Bu, Ph, R'=Me, Et,  $Me_3Si$  n=0, 1), based on crossmetathesis of vinyltrialkoxy- and vinyltris(trimethylsiloxy)silanes with vinyl and allyl, t-butyl (phenyl) sulfides catalyzed by the second generation Grubbs catalyst.

$$SR' + SiR_3 \xrightarrow{[Ru=C]} R_3Si_n$$

$$R_3 = (OEt)_{3}$$
,  $Me_{3}$ ,  $Me_2Ph$   
 $n = 0$  R' = t-Bu, Et, Ph;  
 $n = 1$  R' = t-Bu, Ph

# Stanisław Pasynkiewicz, Ewa Olędzka, Antoni Pietrzykowski

Journal of Molecular Catalysis A: Chemical 224 (2004) 117

Polymerization of alkynes on nickelocene based catalysts: considerations on polymerization mechanism

Novel nickelocene based catalysts were used for polymerization of 2-butyne, 1-phenyl-1-propyne, bis(trimethylsilyl)acetylene and trimethylsilylacetylene. An active catalytic species of polymerization appeared to be {CpNiR} stabilized by alkyne molecule. Cyclization is catalyzed by {CpNiH} species.

$$CpNi \xrightarrow{R} CR' \xrightarrow{R^1C \equiv CR^1} \left\{ CpNi - C = C - R \right\}$$

### Kenton B. Renkema, Ulrike Werner-Zwanziger, Mark D. Pagel, Kenneth G. Caulton

Journal of Molecular Catalysis A: Chemical 224 (2004) 125

Room-temperature hydrosilylation of the C-F bond of vinyl fluoride catalyzed by osmium hydrides

# Patrick W. Blosser, Judith C. Gallucci, Andrew Wojcicki

Journal of Molecular Catalysis A: Chemical 224 (2004) 133

A study of *syn–anti* isomerism of six-coordinate ruthenium(II) complexes containing PhP(CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>PCy<sub>2</sub>)<sub>2</sub> (Cyttp) ligand

The syn and anti isomers of  $[mer\text{-Ru}(\kappa^2\text{-O}_2\text{CX})(\text{CO})(\text{Cyttp})]^n$  (n=0, X=O; n=+1, X=Me, Ph, OMe, OEt) and  $cis\text{-}mer\text{-Ru}X_2(\text{CO})(\text{Cyttp})$  (X=I or Cl) were synthesized and found to be configurationally stable with respect to isomerization and upon ligand substitution. This stability contrasts with that of previously studied related ruthenium(II) Cyttp complexes containing weakly coordinating ligands.

# R.P.J. Bronger, J.P. Bermon, J.N.H. Reek, P.C.J. Kamer, P.W.N.M. van Leeuwen, D.N. Carter, P. Licence, M. Poliakoff

Journal of Molecular Catalysis A: Chemical 224 (2004) 145

The immobilisation of phenoxaphosphine-modified xanthene-type ligand on polysiloxane support and application thereof in the hydroformylation reaction

The rhodium catalysed hydroformylation of 1-octene using a novel heterogenised Xantphos-type ligand is presented. The catalyst shows a high selectivity and stability during hydroformylation studies in both toluene and supercritical carbon dioxide. The catalyst can be recovered by simple phase separation and recycled without significant changes in activity and selectivity.

Silica O Si 
$$\stackrel{\circ}{\downarrow}$$
 O  $\stackrel{\circ}{\downarrow}$  O  $\stackrel{\circ}{\downarrow}$  POP  $\stackrel{\circ}{\downarrow$ 

Silica-1 / Sol-gel-1

#### J. Haber, K. Pamin, J. Połtowicz

Journal of Molecular Catalysis A: Chemical 224 (2004) 153

Cationic metalloporphyrins and other macrocyclic compounds in zeolite matrix as catalysts for oxidation with dioxygen Cationic iron, cobalt and manganese porphyrins, cobalt salen and cobalt phthalocyanine catalysts and these metallocomplexes encapsulated inside zeolite NaX supercages were investigated in oxidation of cyclooctane with molecular oxygen (as air) to cyclooctanone and cyclooctanol without the use of sacrificial co-reductant. We have found that the catalytic activity of catalysts depends on the structure of macrocyclic ring and the type of metal. The product yields and the selectivity to ketone and alcohol are strongly modified by encapsulation in the zeolite matrix.

# Petr Štěpnička, Jan Demel, Jiří Čejka

Journal of Molecular Catalysis A: Chemical 224 (2004) 161

Preparation and catalytic application of MCM-41 modified with a ferrocene carboxyphosphine and a ruthenium complex

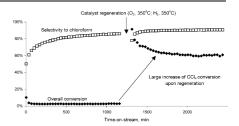
MCM-41 molecular sieves modified with Hdpf and/or,  $[\{Ru(\eta^6\text{-}p\text{-}cymene)Cl(\mu\text{-}Cl)\}_2]$  and the molecular compound **2** were used as catalysts for the reaction between propargyl alcohol and benzoic acid to give 2-oxopropyl benzoate.

# M. Legawiec-Jarzyna, A. Śrębowata, W. Juszczyk, Z. Karpiński

Journal of Molecular Catalysis A: Chemical 224 (2004) 171

Hydrodechlorination of dichlorodifluoromethane, carbon tetrachloride and 1,2-dichloroethane over Pt/Al<sub>2</sub>O<sub>3</sub> catalysts

Alumina-supported platinum is an efficient catalyst in  $CCl_4$  hydrodechlorination (HdCl) to chloroform, whereas in HdCl of  $CCl_2F_2$  and 1,2-dichloroethane this metal exhibits rather low activity. A partial removal of post-reaction residues from the catalyst by oxidative pretreatment brings about a substantial increase of the overall conversion level in  $CCl_4$  hydrodechlorination. Temperature-programmed experiments suggest that a partial removal of coke leads to the formation of very active catalyst, less susceptible to poisoning by chlorine.

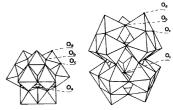


## A. Bielański, A. Lubańska

Journal of Molecular Catalysis A: Chemical 224 (2004) 179

FTIR investigation on Wells-Dawson and Keggin type heteropolyacids: dehydration and ethanol sorption

The changes in the secondary structure on dehydration, of Wells–Dawson and Keggin type heteropolyacids,  $H_6P_2W_{18}O_{62}$  and  $H_3PW_{12}O_{40}$ , as well as during the sorption of ethanol, were observed using FTIR spectroscopy. Frequency of peaks indicates stronger hydrogen bonds formed in the Wells–Dawson type secondary structure than in that of Keggin type one. Sorption of ethanol leads to protonation of  $C_2H_3OH$  molecules and the formation of secondary structure involving ethoxonium ions forming hydrogen bonds between HPA anions.



Keggin and Dawson type HPAs

Patrícia M. Reis, José Armando L. Silva, João J.R. Fraústo da Silva, Armando J.L. Pombeiro

Journal of Molecular Catalysis A: Chemical 224 (2004) 189

Peroxidative oxidation of benzene and mesitylene by vanadium catalysts

Benzene and mesitylene undergo peroxidative oxidation by vanadium (IV and V) catalysts with *N*,*O*-ligands, like *Amavadine* models and related ones, to give, at room temperature, phenol and 3,5-dimethylbenzaldehyde, respectively.

#### Alexander Theodoridis, Rudi van Eldik

Journal of Molecular Catalysis A: Chemical 224 (2004) 197

The role of positively charged meso-substituents on the kinetics of the reductive nitrosylation of iron(III)-porphyrins. The catalytic role of nitrite The cationic  $[Fe^{II}(TMPyP)(H_2O)_2]^{5+}$  porphyrin reacts dissociatively with NO to form  $[Fe^{II}(TMPyP)(H_2O)(NO^+)]^{5+}$ . This species can react with nitrite, to form  $[Fe^{II}(TMPyP)(H_2O)(NO^{\bullet})]^{5+}$ . Concentration, temperature and pressure dependences for the "on" and "off" reaction, as well as for the subsequent reaction with nitrite were studied to clarify the underlying reaction mechanism.

Maria D.M.C. Ribeiro da Silva, Jorge M. Gonçalves, Ana L.R. Silva, Paula C.F.C. Oliveira, Bernd Schröder, Manuel A.V. Ribeiro da Silva

Journal of Molecular Catalysis A: Chemical 224 (2004) 207

Molecular thermochemical study of Ni(II), Cu(II) and Zn(II) complexes with *N,N'*-bis(salicylaldehydo)ethylenediamine

M = Cu(II), Ni(II); Zn(II)

ML = [Cu(salen)], [Ni(salen)]and [Zn(salen)]

# Qingbin Liu, Zhanhui Zhang, Fred van Rantwijk, R.A. Sheldon

Journal of Molecular Catalysis A: Chemical 224 (2004) 213

Osmium-catalyzed asymmetric dihydroxylation of olefins in ionic liquids. The effect of the chiral ligand structure on recyclability

The osmium-catalyzed hydroxylation of *trans*-stilbene in aqueous acetone-ionic liquid medium was enantioselective (85% ee) in the presence of the chiral ligand (D<sub>2</sub>OHQ)<sub>2</sub>PHAL. The chiral ligand was formed from a precursor under the reaction conditions and was recycled together with the ionic liquid.

# Renata Matusiak, Yves Castanet, André Mortreux

Journal of Molecular Catalysis A: Chemical 224 (2004) 217

Dimerisation of butadiene catalyzed by nickel-tris[(1H,1H,2H,2H-perfluorodecyl)phenyl]phosphites complexes in fluorocarbon-hydrocarbon biphasic medium

Triarylphosphites bearing long chain fluorous ponytails have been tested in nickel-based cyclodimerisation of butadiene under fluorous biphasic conditions. *Ortho*-substituted ligands were found as the most effective in terms of activity, selectivity and stability. Recycling experiments of the catalytic system are also reported.

L = Fluorous triarylphosphite