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Articles

Tamás Horváth, József Kaizer, Gábor Speier

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Functional phenoxazinone synthase models. Kinetic studies on the copper-catalyzed oxygenation of 2-aminophenol 2-Aminophenol readily undergoes highly selective Cu-catalyzed oxygenation to 2-aminophenoxazine-3-one.

A.C. Serra, E.C. Marçalo, A.M.d'A. Rocha Gonsalves

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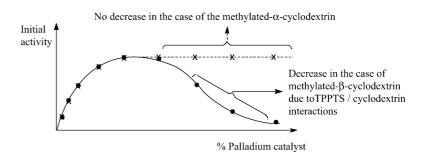
A view on the mechanism of metalloporphyrin degradation in hydrogen peroxide epoxidation reactions

The competition between an intramolecular and an intermolecular mechanism of the catalyst degradation in hydrogen peroxide oxidations is clarified.

Cécile Binkowski, Jérôme Cabou, Hervé Bricout, Frédéric Hapiot, Eric Monflier

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Cleavage of water-insoluble alkylallylcarbonates catalysed by a palladium/TPPTS/cyclodextrin system: effect of phosphine/cyclodextrin interactions on the reaction rate Effect of TPPTS / methylated cyclodextrin interactions on the cleavage rate of allylic substrates as a function of catalyst concentration:

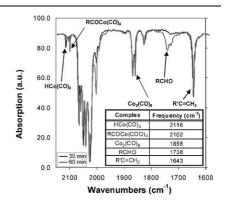


Rina Tannenbaum, György Bor

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Re-evaluation of the mechanism of the stoichiometric hydroformylation of olefins with cobalt carbonyls as catalysts

Two types of stoichiometric hydroformylation reactions have been described in the literature, and have been assumed to proceed via similar mechanisms. Using a high pressure-high temperature infrared throughput cell, we have examined the similarities and discrepancies between the two systems, and offer a new approach to the understanding of these reactions.



Ismail Özdemir, Serpil Demir, Bekir Çetinkaya

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Synthesis of novel rhodium-carbene complexes as efficient catalysts for addition of phenylboronic acid to aldehydes

Rina Ghosh, Swarupananda Maiti, Arijit Chakraborty, Rajkumar Halder

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Indium triflate: a reusable catalyst for expeditious chemoselective conversion of aldehydes to acylals A mild, efficient and expeditious method has been developed for the chemoselective conversion of aldehydes to the corresponding acylals in excellent yields, using acetic anhydride in the presence of catalytic amount (0.01–0.1 mol%) of In(OTf)₃. Ketones remain unaffected under the reaction condition. In(OTf)₃ can be recovered and reused without any loss of its catalytic activity.

RCHO
$$\frac{\text{Ac}_2\text{O (1.2-1.5 equiv), neat / CH}_2\text{Cl}_2}{0.01\text{-}0.1 \text{ mol}\% \text{ In(OTf)}_3, \text{ amb. temp.}}$$
RCH(OAc)₂

$$82\text{-}99\%$$

Hashem Sharghi, Mohammad Mehdi Eskandari, Raoof Ghavami

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A facile conversion of epoxides to halohydrins with elemental halogen using isonicotinic hydrazide (isoniazide) as a new catalyst

Cat = Isoniazide

 $R = Ph, PhOCH_2, H_{13}C_6, CH_2Cl, CH_2BrX = I, Br$

Andrea Vavasori, Luigi Toniolo, Gianni Cavinato

Journal of Molecular Catalysis A: Chemical 215 (2004) 63

Carbon monoxide–ethylene copolymerisation catalysed by $[PdCl_2(dppp)]$ in methanol–water or in acetic acid–water as solvents (dppp = 1,3-bis-(diphenylphosphine)propane)

The complex [PdCl₂(dppp)] yields a perfectly alternated polyketone in MeOH–H₂O (H₂O = 20% (mol/mol), 4100 kg/(g Pd h) at 45 atm and 90 °C) or in AcOH–H₂O (H₂O = 55%, ca. 28 000 kg/(g Pd h)) as solvents. In MeOH–H₂O keto–ester, ester–ester or keto–keto end-groups are observed whereas in AcOH–H₂O, the polyketone shows only keto–keto end-groups. A mechanism for their formation is proposed and the role of H₂O and of the acid in the formation of active species has been explained.

CO +
$$C_2H_4$$

[PdCl₂(dppp)]

H₂O-AcOH

I, II and III

H₂O-AcOH

Celia Z. Flores-López, Lucía Z. Flores-López, Gerardo Aguirre, Lars H. Hellberg, Miguel Parra-Hake, Ratnasamy Somanathan

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Ruthenium(II)-assisted asymmetric hydrogen transfer reduction of acetophenone using chiral tridentate phosphorus-containing ligands derived from (1*R*,2*R*)-1,2-diaminocyclohexane

Several chiral and unsymmetrical tridentate [NNP]-type ligands with sp^2 -N and sp^3 -N were synthesized from optically pure (1R,2R)-1,2-diaminocyclohexane. Their ruthenium(II) complexes have been used as enantioselective catalysts for the asymmetric proton transfer reduction of acetophenone with enantioselectivities in the range 14–99% e.e.

$$\begin{array}{c} \text{CH}_{3} & \text{Ligand,} \\ \text{Ru}(\text{PPh}_{3})_{3}\text{Cl}_{2} \\ \text{HO-} & \text{KOH} \end{array}$$

Véronique Balland, Delphine Mathieu, Nathalie Pons-Y-Moll, Jean François Bartoli, Frédéric Banse, Pierrette Battioni, Jean-Jacques Girerd, Daniel Mansuy

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Non-heme iron polyazadentate complexes as catalysts for oxidations by H_2O_2 : particular efficiency in aromatic hydroxylations and beneficial effects of a reducing agent

Iron(II) polyazadentate complexes catalyze the hydroxylation of aromatic compounds by H_2O_2 . Addition of appropriate reducing agents (hydroquinones, PhSH or tetrahydropterins) led to important increases of the yields based on H_2O_2 (up to 69, 33, 18, 40 and 47% in the case of anisole, toluene, ethylbenzene, benzene and naphthalene, respectively).

Cedric Rabeyrin, Denis Sinou

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Palladium-catalyzed asymmetric arylation of 2,3dihydrofuran with aryl triflates in water in the presence of surfactants

$$Ar = 4-CIC_6H_4$$
, C_6H_5 , $CH_3OC_6H_4$, 1-naphtyl

Ludmila Leite, Vladislavs Stonkus, Kristine Edolfa, Luba Ilieva, Donka Andreeva, Ludmila Plyasova, Janusz W. Sobczak, Sorana Ionescu, Gabriel Munteanu

Journal of Molecular Catalysis A: Chemical 215 (2004) 95

Active phases of supported cobalt catalysts for 2,3-dihydrofuran synthesis

The reaction was studied on kaolin-supported Co and Co–Au catalysts in the liquid phase. It could be suggested that the both ${\rm Co}^0$ and ${\rm Co}^{2+}$ phases in the appropriate ratios are involved in dehydrogenation of 1,4-butanediol into 4-hydroxybutanal intermediate. Catalytic test and XRD analysis show that the presence of metallic cobalt with hexagonal structure is favorable for the selectivity to 2,3-dihydrofuran.

$$\begin{array}{c}
CH_2\text{-}CH_2\text{-}OH & \xrightarrow{\text{cat.}} CH_2\text{-}CHO \\
CH_2\text{-}CH_2\text{-}OH & \xrightarrow{\text{-}} H_2O
\end{array}$$

$$CH_2\text{-}CH_2\text{-}OH \xrightarrow{\text{-}} CH_2\text{-}OH \xrightarrow{\text{-}} CH_2\text{-}OH \xrightarrow{\text{-}} OH \xrightarrow{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{-} OH \xrightarrow{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{\text{-}} OH \xrightarrow{-} OH \xrightarrow{-}} OH \xrightarrow{-} OH \xrightarrow{-} OH \xrightarrow{-} OH \xrightarrow{-}} OH \xrightarrow{-} OH \xrightarrow{-} OH \xrightarrow{-} OH \xrightarrow{-}} OH \xrightarrow{-} OH \xrightarrow{-} OH \xrightarrow{-} OH \xrightarrow{-}$$

Kaushik Mallick, Mike J. Witcomb, Mike S. Scurrell

Journal of Molecular Catalysis A: Chemical 215 (2004) 103

Simplified single-step synthetic route for the preparation of a highly active gold-based catalyst for CO oxidation

Satya Paul, James H. Clark

Journal of Molecular Catalysis A: Chemical 215 (2004) 107

Structure-activity relationship between some novel silica supported palladium catalysts: a study of the Suzuki reaction

A series of novel silica supported palladium catalysts bearing N–N, N–S and N–O chelating ligands have been prepared and characterized on the basis of STA, BET, DRIFT and XPS. Structure-activity relationship between these catalysts has been discussed on the basis of DRIFT and XPS data.

$R = H, CH_3; X = N, O, S$ Catalysts

Nuna C.P. Araújo, Amadeu F. Brigas, M. Lurdes S. Cristiano, Luís M.T. Frija, Emanuel M.O. Guimarães, Rui M.S. Loureiro

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Heteroaromatic benzyl ethers as intermediates for palladium-catalysed transfer hydrogenolysis of benzyl alcohols

K.S. Anisia, G.S. Mishra, A. Kumar

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Reforming of *n*-hexane in presence of [1,2-bis-(salicylidene amino)-phenylene]–zirconium complex chemically bound on modified silica gel support

V.R. Choudhary, D.K. Dumbre, B.S. Uphade, V.S. Narkhede

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Solvent-free oxidation of benzyl alcohol to benzaldehyde by *tert*-butyl hydroperoxide using transition metal containing layered double hydroxides and/or mixed hydroxides

Mn, Cu, and Co containing layered double hydroxides and/or mixed hydroxides show good activity and selectivity in the oxidation of benzyl alcohol by TBHP to benzaldehyde in absence of solvent.

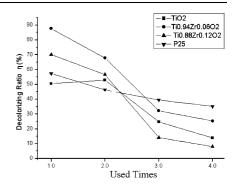
$$CH_2OH + (CH_3)_3COOH$$
 Solid catalyst $OCH_2OH + (CH_3)_3COOH$ CHO + OCH_3OH CHO + OCH_3O

Yan Min Wang, Su Wen Liu, Meng Kai Lü, Shu Fen Wang, Feng Gu, Xue Zhou Gai, Xiao Peng Cui, Jie Pan

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Preparation and photocatalytic properties of Zr⁴⁺-doped TiO₂ nanocrystals

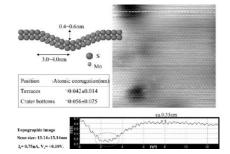
The photocatalytic property of the Zr^{4+} -doped powders is not only higher than that of the pure TiO_2 , but also higher than that of Degussa P_{25} .



Masaharu Komiyama, Kohei Kiyohara, Yanjun Li, Takashi Fujikawa, Takeshi Ebihara, Takeshi Kubota, Yasuaki Okamoto

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Crater structures on a molybdenite basal plane observed by ultra-high vacuum scanning tunneling microscopy and its implication to hydrotreating Crater structures were observed on a natural molybdenite basal plane by STM. Atomic structure was continuous from the surrounding terrace to the crater bottom, with no steps at the rim of the crater. Atomic corrugations were higher at the crater bottoms than on the terraces, indicating higher electronic density of states in the craters.

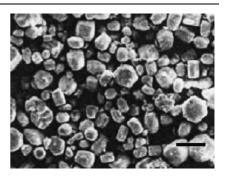


S. Seelan, A.K. Sinha

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Crystallization and characterization of high silica silicoaluminophosphate SAPO-5

SAPO-5 with a high Si content, synthesized by using dipropylamine as a template in ethylene glycol show higher activity for toluene alkylation reaction than samples prepared from the gel with up to 0.6 molar ratio of silica.



J. Araña, J.M. Doña-Rodríguez, O. González-Díaz, E. Tello Rendón, J.A. Herrera Melián, G. Colón, J.A. Navío, J. Pérez Peña

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Gas-phase ethanol photocatalytic degradation study with ${\rm TiO_2}$ doped with Fe, Pd and Cu

During the gas-phase ethanol photocatalytic degradation in a continuos flow system, bare-TiO $_2$ and Fe-TiO $_2$ are deactivated in opposition to what was observed for Pd-TiO $_2$ and Cu-TiO $_2$. Pd and Cu oxide deposits can be capturing the photogenerated electrons, thus avoiding the formation of $O_2^{\bullet-}$ radicals that generate acetates.

Gianguido Ramis, M. Angeles Larrubia

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An FT-IR study of the adsorption and oxidation of N-containing compounds over Fe_2O_3/Al_2O_3 SCR catalysts

On Fe_2O_3/Al_2O_3 SCR catalyst hydrazine can be intermediate in the oxidation of ammonia to nitrogen, while hydroxylamine-type species, can be intermediate in the oxidation of ammonia to NO, on contrary to those over Fe_2O_3/TiO_2 indicating that Fe_2O_3/Al_2O_3 is less selective in SCR reaction with ammonia.

Animonia Urea
$$\begin{array}{c} N_{0} \\ N_{1} \\ N_{1} \\ N_{1} \\ N_{2} \\ N_{3} \\ N_{4} \\ N_{5} \\ N_{5} \\ N_{7} \\ N_{8} \\ N_{8} \\ N_{1} \\ N_{2} \\ N_{3} \\ N_{4} \\ N_{5} \\ N_{5} \\ N_{5} \\ N_{6} \\ N_{7} \\ N_{8} \\$$

Sujit Samanta, Nawal Kishor Mal, Prashant Kumar, Asim Bhaumik

Journal of Molecular Catalysis A: Chemical 215 (2004) 169

Hydrothermally synthesized high silica mordenite as an efficient catalyst in alkylation reaction under liquid phase condition High silica mordenite samples have been synthesized hydrothermally using low aluminum contents (Si/Al molar ratios 40 and 60 in the gel) in the presence of orthophosphoric acid as promoter. These materials showed excellent catalytic activity and selectivity towards linear alkyl benzenes in the alkylation of bezene using 1-dodecene as alkylating agent under mild liquid phase condition.

$$\frac{\text{High silica MOR}}{353 \text{ K, Liquid phase}} + \frac{\text{High silica MOR}}{353 \text{ K, Liquid phase}}$$

Helen L. Ngo, Aiguo Hu, Wenbin Lin

Journal of Molecular Catalysis A: Chemical 215 (2004) 177

Molecular building block approaches to chiral porous zirconium phosphonates for asymmetric catalysis

Chiral porous solids based on BINOL-derived Zr phosphonates have been synthesized via a molecular building block approach, whose dihydroxy functionalities coordinate to Ti(IV) centers to form active catalysts for the asymmetric additions of diethylzinc to aromatic aldehydes with high conversions and e.e. values of up to 72%.

A. Góra, E. Brocławik

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Theoretical estimation of acid-base properties of Lewis and Brønsted centres at the V-W-O catalyst surface: water molecule as the probe in DFT calculations Water molecule adsorbed on models of active sites postulated on the surface of V-W-O catalysts served as a probe for sites acidity and basicity. Geometry, OH stretching frequencies and water binding energy were chosen as three computed parameters to characterise the Lewis acid and basic sites and Brønsted acid sites situated in varying environment.

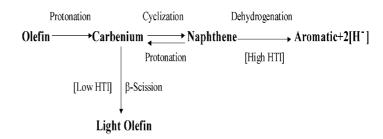


Conghua Liu, Youquan Deng, Yuanqing Pan, Yusheng Gu, Botao Qiao, Xionghou Gao

Journal of Molecular Catalysis A: Chemical 215 (2004) 195

Effect of ZSM-5 on the aromatization performance in cracking catalyst

Journal of Molecular Catalysis A: Chemical; reaction pathways over ZSM-5 zeolite contained FCC catalyst in catalytic cracking reaction.



V.N. Sheemol, Beena Tyagi, Raksh V. Jasra

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Acylation of toluene using rare earth cation exchanged zeolite β as solid acid catalyst

The catalytic activity of rare earth cations exchanged zeolite β was studied for the acylation of toluene with acetic anhydride as an acylating agent in the liquid phase. The correlation of catalytic activities of the different catalysts with the cyclohexanol dehydration as well as DRIFT spectroscopy showed that the toluene acylation is a Brönsted acid catalyzed reaction.