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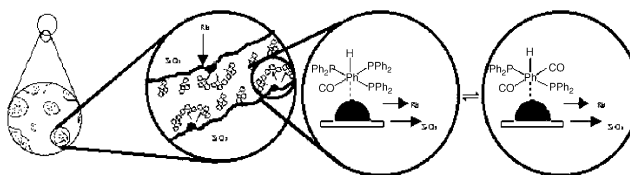
Articles

**Li Yan, Yun J. Ding, He J. Zhu, Jian M. Xiong,
Tao Wang, Zhen D. Pan, Li W. Lin**

Journal of Molecular Catalysis A: Chemical 234
(2005) 1

Ligand modified real heterogeneous catalysts for
fixed-bed hydroformylation of propylene

A novel heterogeneous $\text{PPh}_3\text{-Rh/SiO}_2$ catalyst showing high activity and selectivity under mild conditions (1 MPa, 393 K) has been developed; the problem of metal leaching is greatly reduced and no sign of deactivation is observed over a period of more than 1000 h.

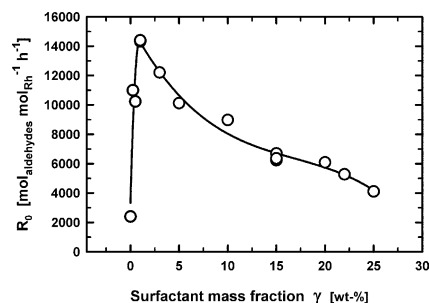


**Christian C. Miyagawa, Jörg Kupka,
Adrian Schumpe**

Journal of Molecular Catalysis A: Chemical 234
(2005) 9

Rhodium-catalyzed hydroformylation of 1-octene
in micro-emulsions and micellar media

The initial rate of aldehyde formation referred to moles of rhodium, R_0 , runs through a sharp maximum at about the critical micelle concentration of non-ionic surfactant (Lutensol[®] ON 70).

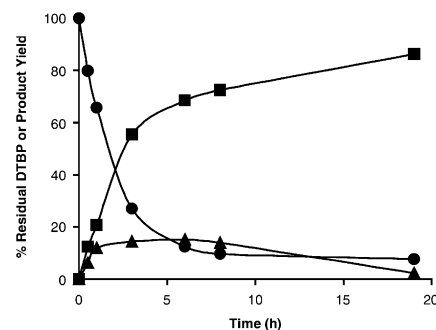


Hayrettin Türk, Yasemin Çimen

Journal of Molecular Catalysis A: Chemical 234
(2005) 19

Oxidation of 2,6-di-*tert*-butylphenol with *tert*-butylhydroperoxide catalyzed by cobalt(II) phthalocyanine tetrasulfonate in a methanol–water mixture and formation of an unusual product 4,4'-dihydroxy-3,3',5,5'-tetra-*tert*-butylbiphenyl

Cobalt(II) phthalocyanine tetrasulfonate catalyzed oxidation of 2,6-di-*tert*-butylphenol (●) with *tert*-butylhydroperoxide in a 80% methanol–water mixture yields predominantly the coupled products 3,3',5,5'-tetra-*tert*-butyl-4,4'-diphenoquinone (■) and 4,4'-dihydroxy-3,3',5,5'-tetra-*tert*-butylbiphenyl (▲) when the oxidant/substrate ratio was less than 10.

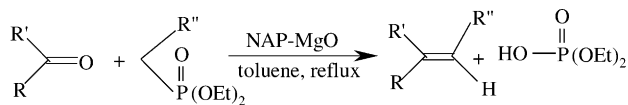


**Boyapati Manoranjan Choudary,
Koosam Mahendar, Kalluri Venkata
Sri Ranganath**

Journal of Molecular Catalysis A: Chemical 234
(2005) 25

Wadsworth–Emmons reactions catalyzed by nano-
crystalline MgO

The Wadsworth–Emmons reaction between aldehydes (aliphatic, aromatic, cyclic or heterocyclic) and phosphonates to afford α,β -unsaturated nitriles and esters under mild conditions without the formation of by-products, using nanocrystalline MgO as a catalyst is described.



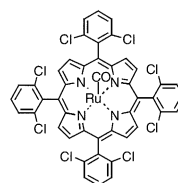
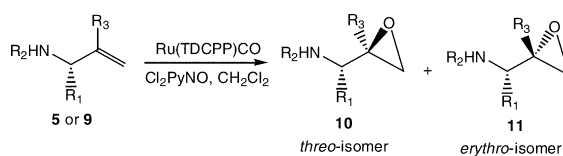
R = aryl, alkyl, cyclohexyl, furfuryl
R' = H

2a: R'' = COOEt
2b: R'' = COOMe
2c: R'' = COO'Bu
2d: R'' = CN
2e: R'' = Cl

**Li Sun, Can-Ping Du, Jie Qin, Jing-Song You,
Meng Yang, Xiao-Qi Yu**

Journal of Molecular Catalysis A: Chemical 234
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Highly diastereoselective epoxidation of protected
 α -amino alkenes catalyzed by ruthenium por-
phyrin/ Cl_2PyNO system



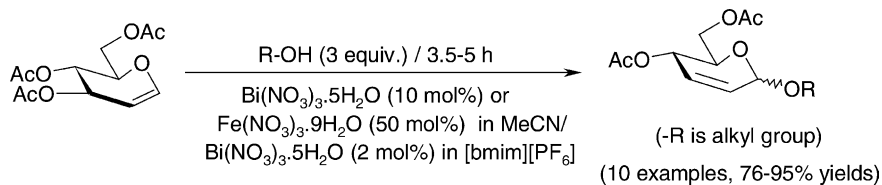
Ru(TDCPP)CO

**Prashant U. Naik, Susheel J. Nara,
Jitendra R. Harjani, Manikrao M. Salunkhe**

Journal of Molecular Catalysis A: Chemical 234
(2005) 35

Metal nitrates catalysed *O*-glucosylation using
acetyl glucal in organic solvents and ionic liquids:
A comparative investigation

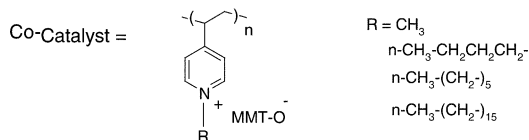
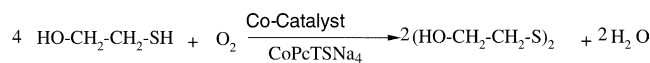
The screening of metal nitrates revealed the ability of $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ and $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ as catalyst for the Ferrier *O*-glucosylation using 3,4,6-tri-*O*-acetyl- D -glucal. The $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ -mediated *O*-glucosylation show substantial solvent dependency and enhanced reaction rate in [bmim][PF₆] than in the conventional organic solvents. Apart from the ambient quality, eco-friendly nature and catalyst economy, the $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ /[bmim][PF₆] method offers good yields and high anomeric selectivity, reduced catalyst concentration, reduced reaction time and recyclability of reaction medium.



**M. Hassanein, H. El-Hamshary, N. Salahuddin,
A. Abu-El-Fotoh**

Journal of Molecular Catalysis A: Chemical 234
(2005) 45

Oxidation of 2-mercaptoethanol catalyzed by
cobalt(II) phthalocyaninetetrasulfonate supported
on poly-*N*-alkyl-4-vinyl pyridinium/montmorillo-
nite intercalates

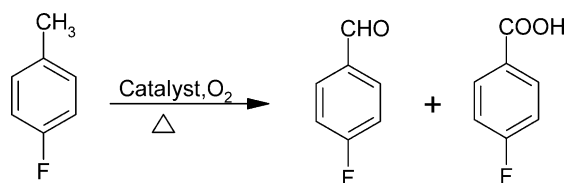


**Sushil K. Maurya, Pratap Patil,
Shubhangi B. Umbarkar, Mukund K. Gurjar,
Mohan Dongare, Stephan Rudiger,
Erhard Kemnitz**

Journal of Molecular Catalysis A: Chemical 234
(2005) 51

Vapor phase oxidation of 4-fluorotoluene over
vanadia–titania catalyst

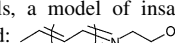
The vapor phase oxidation of 4-fluorotoluene has been carried out over vanadia–titania catalysts with moderate conversion and selectivity for 4-fluorobenzaldehyde. Two series of V_2O_5/TiO_2 catalysts with 1–10 mol% vanadia, prepared by sol–gel and impregnation technique were used for catalytic oxidation.



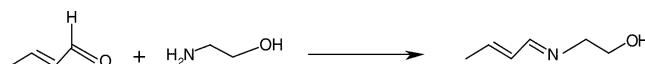
**C. Longuet, B. Coq, R. Durand, A. Finiels,
P. Geneste, M. Mauvezin**

Journal of Molecular Catalysis A: Chemical 234
(2005) 59

Oligomer model to explain the coloration of TEA
and discoloration catalytic treatment

To understand origin of the undesirable well-known coloration of triethanolamine by compounds at trace levels, a model of insaturated oligomers is proposed: . This model is obtained by action of crotonaldehyde on MEA:

The hydrogenation in the presence of various supported metal catalysts is an attractive process for TEA discoloration, and a 5 wt.% Pd/C catalyst exhibited the highest efficiency.

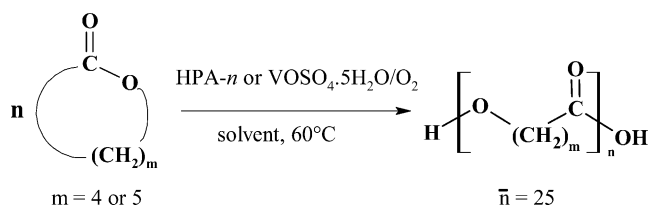


**Yahdih Mahha, Ahmed Atlamsani,
Jean-Claude Blais, Martine Tessier,
Jean-Marie Brégeault, Laurent Salles**

Journal of Molecular Catalysis A: Chemical 234
(2005) 63

Oligomerization of ϵ -caprolactone and δ -valerolactone using heteropolyacid initiators and vanadium or molybdenum complexes

Preparation of the oligomers of ϵ -caprolactone and δ -valerolactone having reactive functional groups, such as hydroxyl and carboxyl groups, were studied in the presence of “heteropolyacids/ O_2 /solvent” or “ $VOSO_4 \cdot 5H_2O/THF-H_2O/O_2$ ” systems. These oligomers were characterized by various physicochemical techniques.



**Run Xu, Wei Wei, Wen-huai Li, Tian-dou Hu,
Yu-han Sun**

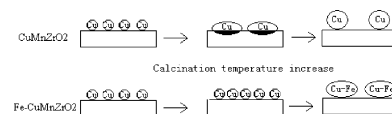
Journal of Molecular Catalysis A: Chemical 234
(2005) 75

Fe modified $CuMnZrO_2$ catalysts for higher alcohols synthesis from syngas: Effect of calcination temperature

The effect of iron on the structure and catalytic performance was investigated by comparison of iron-promoted and un-promoted catalysts calcined at different temperature. It was found that, when the catalysts were calcined at different temperature, the change of metal-support interaction

strongly influenced the surface and crystal structure of the catalysts and hence its catalytic performance. Low calcination temperature yielded poorly crystallized catalysts and favored the formation of a $Cu(OH)_2$ -like structure, which was highly dispersed. For the $CuMnZrO_2$ catalyst, with the rise of calcination temperature, surface area and dispersion of copper decreased, and the crystallization of zirconia occurred. Nevertheless, the TOF showed a maximum on the catalyst calcined at 873K due to the increase of the copper–zirconia interaction. The presence of iron could suppress agglomeration of copper species and crystallization of amorphous zirconia. The dispersion of copper was enhanced. However, overall catalytic activity was suppressed. On the one hand, the

increase of iron–zirconia interaction with the rise of calcination temperature suppressed the interaction between copper species and zirconia. On the other hand, the interaction between iron and zirconia hindered the reduction of iron oxide, and then copper–iron interaction weakened, which reduced the active sites for higher alcohol formation.

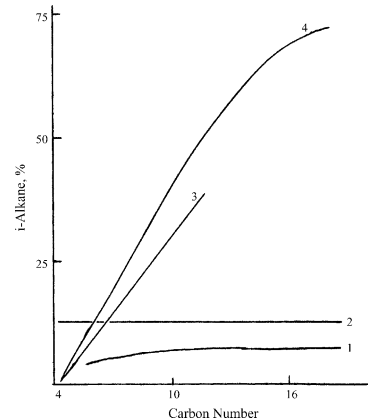


**Buchang Shi, Robert A. Keogh,
Burtron H. Davis**

Journal of Molecular Catalysis A: Chemical 234
(2005) 85

Fischer–Tropsch synthesis: The formation of branched hydrocarbons in the Fe and Co catalyzed reaction

The fraction of *iso*-alkanes depends upon reaction temperature. Increasing amounts of K with an iron catalyst leads to increasing fraction of *iso*-alkanes. Iron catalysts produce more *iso*-alkanes than cobalt catalysts.

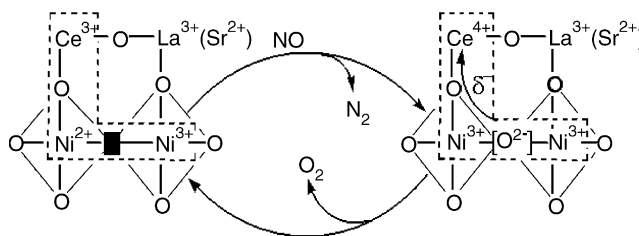


**Junjiang Zhu, Dehai Xiao, Jing Li,
Xiangguang Yang, Yue Wu**

Journal of Molecular Catalysis A: Chemical 234
(2005) 99

Effect of Ce on NO direct decomposition in the absence/presence of O₂ over La_{1-x}Ce_xSrNiO₄ (0 ≤ x ≤ 0.3)

Ce added catalysts La_{1-x}Ce_xSrNiO₄ (0 ≤ x ≤ 0.3) showed high activity for NO decomposition even in the presence of excess oxygen, due to the formation of the new highly active site: Ce³⁺-(O)-(Ni²⁺-[]-Ni³⁺).

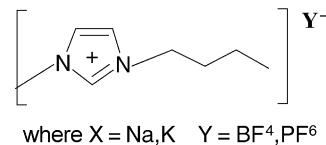


**Trissa Joseph, Suman Sahoo,
S.B. Halligudi**

Journal of Molecular Catalysis A: Chemical 234
(2005) 107

Brønsted acidic ionic liquids: A green, efficient and reusable catalyst system and reaction medium for Fischer esterification

Brønsted acidic ionic liquid containing nitrogen-based organic cations 1-methylimidazole and 1-butyl-3-methylimidazolium and inorganic anions of the type BF₄⁻, PF₆⁻ and PTSA⁻ has been synthesized in good yields and used as a catalysts and reaction medium for Fischer esterification of alcohols with acids.

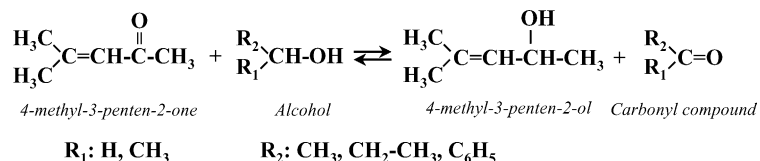


J.I. Di Cosimo, A. Acosta, C.R. Apesteguía

Journal of Molecular Catalysis A: Chemical 234
(2005) 111

Allylic alcohol synthesis by gas-phase hydrogen transfer reduction of unsaturated ketones

Gas-phase reduction of 4-methyl-3-penten-2-one (mesityl oxide) to allylic alcohol was studied on MgO using alcohols as hydrogen donors. Reaction proceeds on the surface Mg²⁺-O²⁻ pairs by a Meerwein–Ponndorf–Verley mechanism. Stability, activity and selectivity of MgO were strongly dependent on the reaction temperature, reactant ratio, contact time, and hydrogen donor.

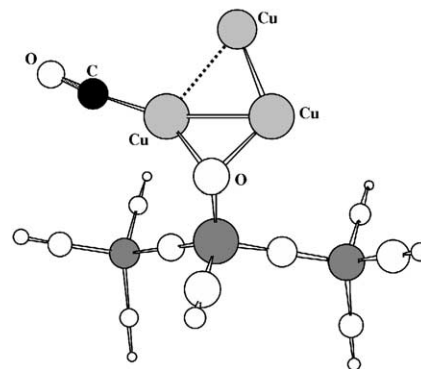


Ricardo M. Ferullo, Norberto J. Castellani

Journal of Molecular Catalysis A: Chemical 234 (2005) 121

A quantum-chemical study of CO adsorption on small Cu particles supported on reduced SiO₂

The adsorption of CO over Cu₁, Cu₂ and Cu₃ deposited on a ≡ SiO–O• defect of silica was studied using DFT. The CO adsorption strength follows this order: Cu₁ > Cu₂ ≥ Cu₃. While for closed-shell systems CO shows the lower frequency shifts, for the open-shell systems the behaviour is the opposite. This could be related with the variation of polarizabilities when CO interacts with Cu_n/SiO₂.



Marta Lasa, Pilar López, Carlos Cativiela, Daniel Carmona, Luis A. Oro

Journal of Molecular Catalysis A: Chemical 234 (2005) 129

Chiral-at-metal ruthenium(II) complexes as catalysts in the asymmetric cyclopropanation reaction

A family of five- and six-coordinate chiral-at-metal ruthenium complexes has been examined as catalysts in the asymmetric cyclopropanation reaction of styrene with ethyl diazoacetate. With complexes **5** and **6**, good *cis*-diastereoselectivity and enantioselectivity up to 74% were observed.

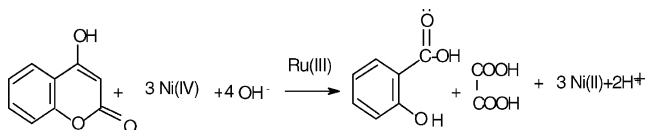


Ramesh S. Shettar, Sharanappa T. Nandibewoor

Journal of Molecular Catalysis A: Chemical 234 (2005) 137

Kinetic, mechanistic and spectral investigations of ruthenium(III)-catalysed oxidation of 4-hydroxycoumarin by alkaline diperiodatonickelate(IV) (stopped flow technique)

The title reaction was studied using spectrophotometer connected to a rapid kinetic accessory. A mechanism involving the formation of complex between 4-hydroxycoumarin and hydroxylated species of ruthenium(III) has been proposed. The product was characterized by IR, NMR, and spot tests.

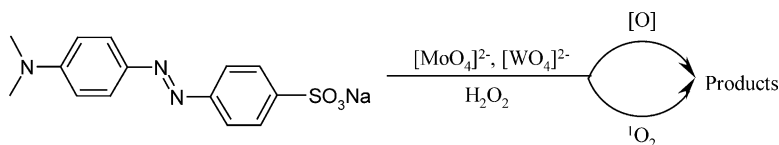


David M. Gould, Michael Spiro, William P. Griffith

Journal of Molecular Catalysis A: Chemical 234 (2005) 145

Mechanism of bleaching by peroxides. Part 6. Kinetics of the peroxide bleaching of methyl orange catalysed by MoO₄²⁻ and WO₄²⁻ at pH 10

Kinetics and mechanisms of the bleaching of methyl orange by H₂O₂ catalysed by MoO₄²⁻ and WO₄²⁻ have been studied. Bleaching arises from two parallel catalytic routes: (a) H₂O₂ oxidation by peroxy complexes, denoted by [O] in the diagram, and (b) singlet oxygen, ¹O₂, also produced by peroxy complexes.

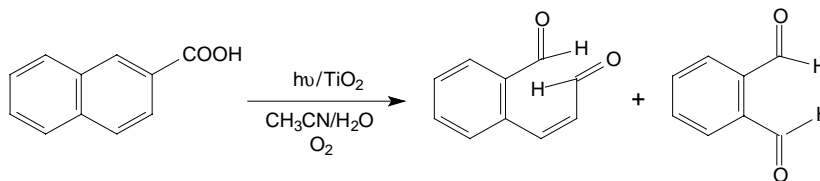


M. Muneer, M. Qamar, D. Bahnemann

Journal of Molecular Catalysis A: Chemical 234 (2005) 151

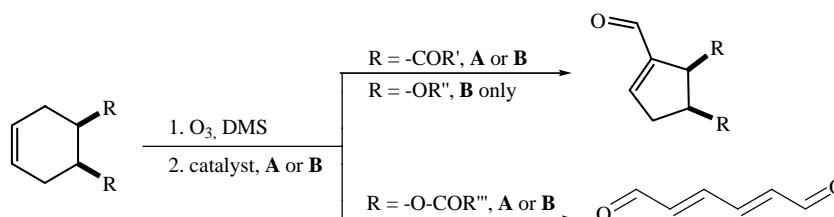
Photoinduced electron transfer reaction of few selected organic systems in presence of titanium dioxide

Photocatalysed reaction of few selected organic systems such as 2-naphthoic acid, 2,6-dichloro-4-nitro aniline (dichloran), 4-nitro phenyl acetate, 1,3-diallyl-2-thio-urea and 7-hydroxy-4-methyl coumarin has been investigated in water or acetonitrile/water mixture in the presence of TiO₂. GC-MS analysis of the irradiated mixture showed the formation of oxidative products. A probable pathway for the formation of products has been proposed involving OH• and O₂^{-•}.

**Vanya B. Kurteva, Carlos A.M. Afonso**

Journal of Molecular Catalysis A: Chemical 234 (2005) 159

A study on the intramolecular catalytic aldol cyclodehydration of 3,4-disubstituted 1,6-dialdehydes

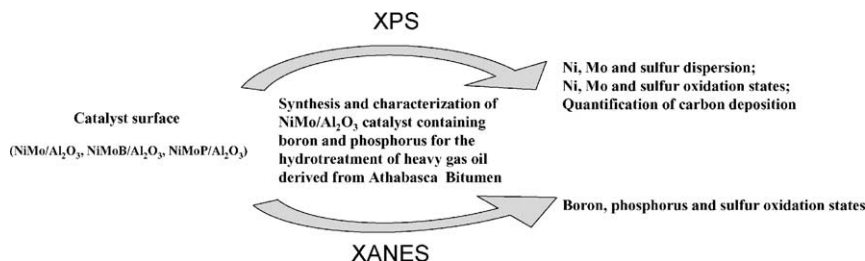


(A) - dibenzylammonium trifluoroacetate; (B) - piperidinium acetate

D. Ferdous, A.K. Dalai, J. Adjaye

Journal of Molecular Catalysis A: Chemical 234 (2005) 169

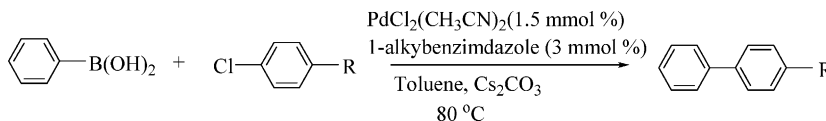
X-ray absorption near edge structure and X-ray photo electron spectroscopy analyses of NiMo/Al₂O₃ catalysts containing boron and phosphorus

**İsmail Özdemir, Neslihan Şahin, Yetkin Gök, Serpil Demir, Bekir Çetinkaya**

Journal of Molecular Catalysis A: Chemical 234 (2005) 181

In situ generated 1-alkylbenzimidazole-palladium catalyst for the Suzuki coupling of aryl chlorides

A convenient method for Suzuki cross-coupling reaction is presented which employs a catalyst formed in situ from PdCl₂(CH₃CN)₂, air stable 1-alkylbenzimidazole.

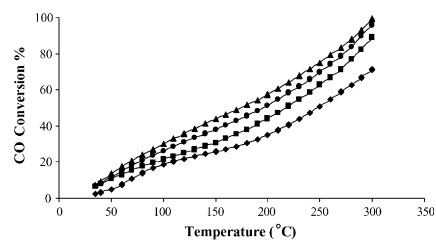


**Iza Dobrosz, Kveta Jiratova,
Véronique Pitchon, Jacek M. Rynkowski**

Journal of Molecular Catalysis A: Chemical 234
(2005) 187

Effect of the preparation of supported gold particles on the catalytic activity in CO oxidation reaction

Gold catalysts supported on hydrotalcite, for CO oxidation reaction, were prepared by Direct Anionic Exchange (DAE) or by deposition-precipitation with NaOH or urea. The highest activity was obtained for Au/Mg₄Al₂ prepared by DAE. The chloride was removed either with warm water or with ammonia. Changes in activity were observed according to the washing procedure.



Effect of washing procedure on CD activity for Au/Mg₄Al₂: without washing (◆), washed in ammonia (●), washed in ammonia 'in situ' (■), washed in warm water (▲).