



## Contents

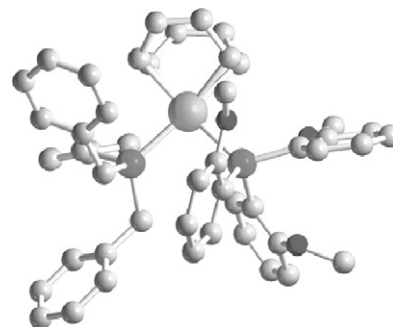
### Articles

**Vanessa R. Landaeta, Francisco López-Linares, Roberto Sánchez-Delgado, Claudio Bianchini, Fabrizio Zanolini, Maurizio Peruzzini**

*Journal of Molecular Catalysis A: Chemical 301 (2009) 1*

Synthesis and characterization of new rhodium and iridium complexes with trianisylphosphine,  $\text{PA}_3$ , and evaluation of their catalytic behavior in the homogeneous hydrogenation of cinnamaldehyde

New rhodium and iridium complexes with the bulky tris(*ortho*-methoxyphenyl)phosphine ( $\text{PA}_3$ ) have been obtained and properly characterized, including X-ray diffraction structures for  $\text{RhCl}(\text{PA}_3)(\text{COD})$  (**1**) and  $[\text{Ir}(\text{PBz}_3)(\text{PA}_3)(\text{COD})]\text{PF}_6$  (**4**). Among the new compounds,  $[\text{Ir}(\text{PA}_3)(\text{py})(\text{COD})]\text{PF}_6$  (**6**) and the analogues with  $\text{PTol}_3$  and  $\text{PBz}_3$  were tested and compared as precursors for the catalytic hydrogenation of *trans*-cinnamaldehyde, observing changes both in activity and selectivity.

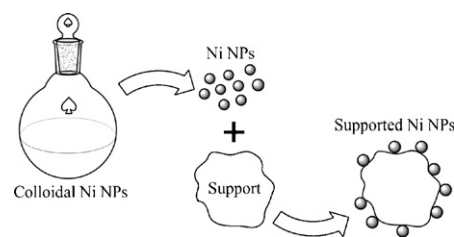


**Roberto Rinaldi, Andréia de Melo Porcari, Tulio C.R. Rocha, Wellington Henrique Cassinelli, Renata Uema Ribeiro, José Maria Correa Bueno, Daniela Zanchet**

*Journal of Molecular Catalysis A: Chemical 301 (2009) 11*

Construction of heterogeneous Ni catalysts from supports and colloidal nanoparticles – A challenging puzzle

To construct heterogeneous Ni catalysts from supports and colloidal Ni nanoparticles is a challenging puzzle. Surprisingly, “1 + 1” is not equal to “the best catalyst”, following this synthetic methodology. The thought-provoking lack of catalytic activity of Ni colloidal NPs supported on silica Aerosil was analyzed in details, and the factors responsible for the low catalytic activity of Ni/ $\text{SiO}_2$  system proposed.



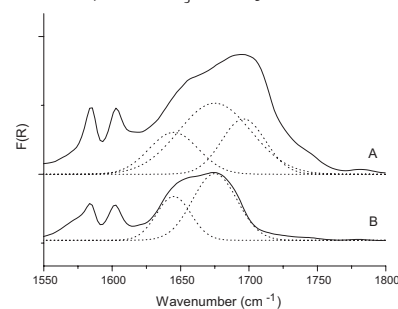
**A.G. Potapov, G.D. Bukatov, V.A. Zakharov**

*Journal of Molecular Catalysis A: Chemical 301 (2009) 18*

DRIFTS study of the interaction of the  $\text{AlEt}_3$  cocatalyst with the internal donor ethyl benzoate in supported Ziegler–Natta catalysts

The internal donors in supported Ziegler–Natta catalysts form several types of complexes on surface of  $\text{MgCl}_2$  support. A part of the internal donors is removed from the catalysts at interaction of the catalysts with  $\text{AlEt}_3$  cocatalyst. IR spectroscopy of diffuse reflection (DRIFTS) was used to study the interaction of the support EB/ $\text{MgCl}_2$  and the catalysts  $\text{TiCl}_4/\text{EB}/\text{MgCl}_2$  (where EB—ethyl benzoate) with  $\text{AlEt}_3$  cocatalyst.

DRIFT spectra of the EB adsorbed on the surface of  $\text{MgCl}_2$  support (before (A) and after (B) interaction with  $\text{AlEt}_3$ ) demonstrating effect of  $\text{AlEt}_3$  on the distribution of EB complexes on  $\text{MgCl}_2$  surface.

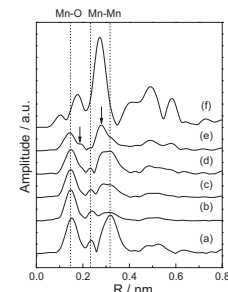


**Qinghu Tang, Xiaona Huang, Yuanting Chen, Tao Liu, Yanhui Yang**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 24

Characterization and catalytic application of highly dispersed manganese oxides supported on activated carbon

Activated carbon supported manganese oxides (Mn/AC) were prepared, the nature of supported manganese oxides was extensively characterized by a variety of techniques. The highly dispersed manganese oxides, uniformly distributed on activated carbon surface mainly as coexistence of  $Mn^{2+}$  and  $Mn^{3+}$ , have been demonstrated to be catalytically active in the aerobic oxidation of benzyl alcohol using molecular oxygen.

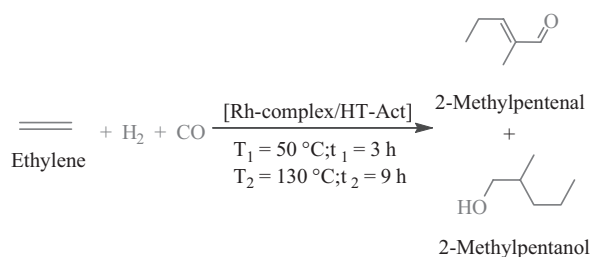


**Sumeet K. Sharma, Parimal A. Parikh, Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 31

Synthesis of 2-methylpentanol from ethylene in single pot using eco-friendly  $HRhCO(PPh_3)_3$  supported on activated hydrotalcite as a multi-functional catalyst

The multi-functional [Rh-complex/HT-Act] catalyst system was synthesized by impregnation of  $HRhCO(PPh_3)_3$  [Rh-complex] on the surface of activated hydrotalcite [HT-Act] for selective synthesis of 2-methylpentanol from ethylene in single pot. The maximum selectivity of 2-ethylpentanol (86%) was observed in polar solvents such as methanol as compared to non-polar solvents toluene (79%).

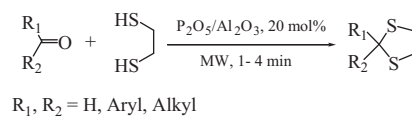


**Amin Zarei, Abdol R. Hajipour, Leila Khazdooz, Bibi F. Mirjalili, Saeed Zahmatkesh**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 39

Fast, efficient and chemoselective method for thioacetalization and transthoacetalization using catalytic amount of  $P_2O_5/Al_2O_3$  under microwave irradiation

A wide variety of aldehydes and ketones can be easily protected to their corresponding 1,3-dithiolanes using 1,2-ethanedithiol in the presence of catalytic amount of  $P_2O_5/Al_2O_3$  under microwave irradiation. Using this method, transthoacetalization of acetals and acylals into their corresponding 1,3-dithiolanes was also carried out in good yields.

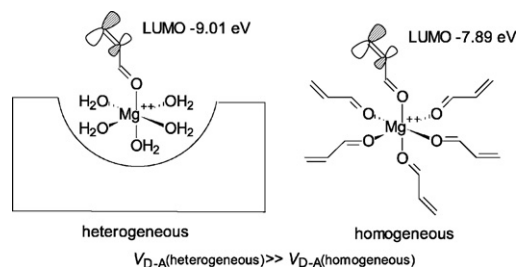


**Ian D. Cunningham, Vanessa Crawley**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 47

Catalysis of the Diels–Alder reaction by solids

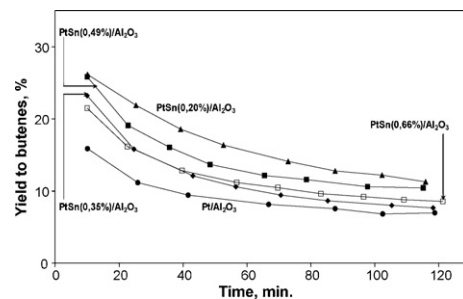
Enhancement of the rate of Diels–Alder reaction by solids such as silica, carbon, magnesium perchlorate and *bis*-resorcinolanthracene can be comparable to, and in the case magnesium perchlorate much greater than, that of homogeneous catalysts.



**Sonia A. Bocanegra, Sergio R. de Miguel, Irina Borbath, Jozsef L. Margitfalvi, Osvaldo A. Scelza**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 52

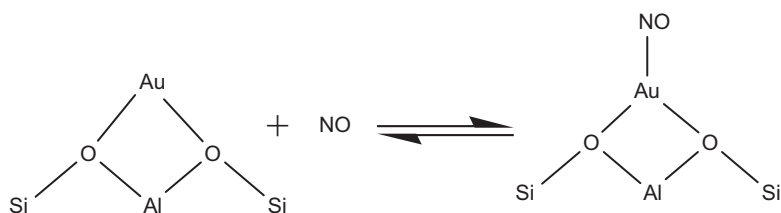
Behavior of bimetallic PtSn/Al<sub>2</sub>O<sub>3</sub> catalysts prepared by controlled surface reactions in the selective dehydrogenation of butane



**Anibal Sierraalta, Paola Alejos, Elena Ehrmann, Leonardo J. Rodriguez, Yetziree Ferrer**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 61

DFT-ONIOM study of Au/ZSM-5 catalyst: Active sites, thermodynamic and vibrational frequencies

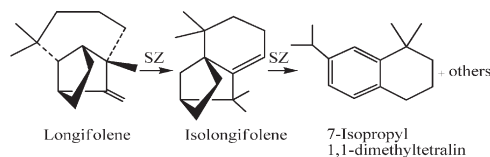


**Beena Tyagi, Manish K. Mishra, Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 67

Solvent free synthesis of 7-isopropyl-1,1-dimethyltetralin by the rearrangement of longifolene using nano-crystalline sulfated zirconia catalyst

Longifolene rearranges to 7-isopropyl-1,1-dimethyltetralin via isolongifolene over nano-crystalline sulfated zirconia (SZ) catalyst.

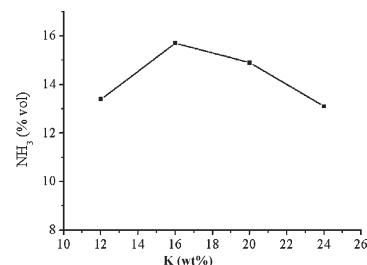


**Ying Zheng, Yong Zheng, Zhaohui Li, Haoying Yu, Rong Wang, Kemei Wei**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 79

Preparations of C/SiC composites and their use as supports for Ru catalyst in ammonia synthesis

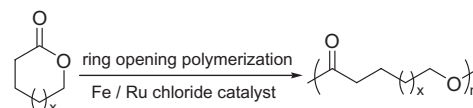
The catalytic activity of the C/SiC-supported Ru catalysts exceeds that of the traditional Fe-based catalyst (ICI-74-1) at lower temperatures. At 435 °C, 10.0 MPa and a N<sub>2</sub>/H<sub>2</sub> (1/3) flow rate of 10 000 h<sup>-1</sup>, the optimum activity of 15.9% ammonia in the effluent can be reached when C/SiC-5 (C/TEOS molar ratio = 5) was used as the catalyst support, with the potassium promoter loaded to 16 wt%.



**Ravikumar R. Gowda, Debashis Chakraborty***Journal of Molecular Catalysis A: Chemical* 301 (2009) 84

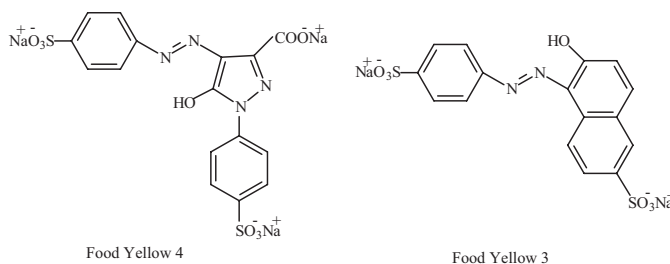
Environmentally benign process for bulk ring opening polymerization of lactones using iron and ruthenium chloride catalysts

Ring opening polymerization of cyclic lactone monomers using iron and ruthenium chloride catalysts is discussed. Such polymerizations constitute an economical process, employing readily available inorganics as catalysts and do not necessitate solvents. The overall system is green and eco friendly.

**Cleci Teresinha Fragoso, Rodrigo Battisti, Crisleide Miranda, Paulo Cesar de Jesus***Journal of Molecular Catalysis A: Chemical* 301 (2009) 93

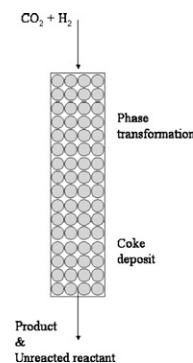
Kinetic of the degradation of C.I. Food Yellow 3 and C.I. Food Yellow 4 azo dyes by the oxidation with hydrogen peroxide

The kinetic of the degradation of Food Yellow 3 (FY3) and Food Yellow 4 (FY4) dyes by oxidation using hydrogen peroxide 30% in alkaline solution was studied. The kinetics were measured spectrophotometrically by UV-vis at 427 nm for FY4 and 485 nm for FY3 and under a temperature range of 25–70 °C. The kinetic activation parameters ( $E_a$ ,  $\Delta H^\ddagger$ ,  $\Delta G^\ddagger$  and  $\Delta S^\ddagger$ ) were calculated.

**Sung-Chul Lee, Jun-Sik Kim, Woo Cheol Shin, Myung-Jae Choi, Suk-Jin Choung***Journal of Molecular Catalysis A: Chemical* 301 (2009) 98

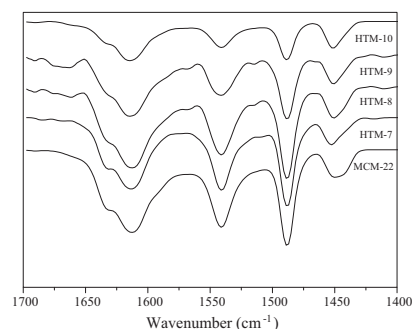
Catalyst deactivation during hydrogenation of carbon dioxide: Effect of catalyst position in the packed bed reactor

The deactivation occurred on Fe-K/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst during the CO<sub>2</sub> hydrogenation. The deactivation pathway was different according to the reactor position. The main deactivation reason at the inlet part in the reactor was phase transformation. Conversely, the main factor at the outlet part in the reactor was the coke deposit generated by secondary reactions.

**Yongxin Li, Bing Xue, Xueyi He***Journal of Molecular Catalysis A: Chemical* 301 (2009) 106

Synthesis of ethylbenzene by alkylation of benzene with diethyl carbonate over parent MCM-22 and hydrothermally treated MCM-22

MCM-22 hydrothermally treated at 873 K exhibits a great improvement in ethylbenzene selectivity along with a slight decrease in benzene conversion, corresponding to the proper acidity strength of the catalyst. It indicates that alkylation of benzene with diethyl carbonate mainly occurred on Brønsted acid sites, and the effect of Lewis acid sites on the alkylation process was negligible.

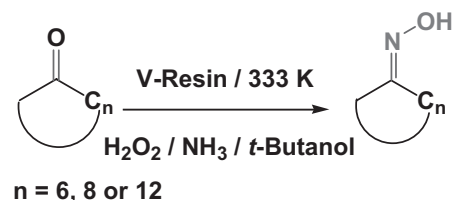


**Sanghamitra Mukherjee, Mahasweta Nandi, Krishanu Sarkar, Asim Bhaumik**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 114

Vanadium resin as an efficient catalyst for the liquid phase ammoxidation of cyclic ketones

A new vanadium resin has been prepared through ion exchange at the cationic sites of Amberlite IR 120 resin and this material showed excellent catalytic activity and selectivity in the ammoxidation of bulky cyclic ketones to their respective oximes in the presence of dilute aqueous  $H_2O_2$  and ammonia.

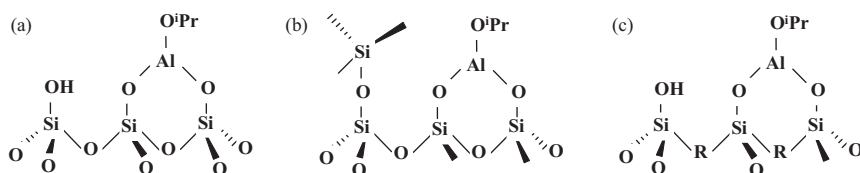


**S. Shylesh, Mahendra P. Kapoor, Lekh. R. Juneja, Prinson P. Samuel, Ch. Srilakshmi, A.P. Singh**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 118

Catalytic Meerwein-Ponndorf-Verley reductions over mesoporous silica supports: Rational design of hydrophobic mesoporous silica for enhanced stability of aluminum doped mesoporous catalysts

Aluminium isopropoxide-grafted mesoporous silicas (MCM-41, MCM-48, SBA-15), silylated mesoporous silicas and organosilicas (having ethane ( $-CH_2-CH_2-$ ) and ethene ( $-CH=CH-$ ) groups in the frame wall positions) were synthesized (see picture) and were applied as catalysts in the MPV reduction reaction of ketones and aldehydes of different nature and size using secondary alcohols as the hydrogen transfer agents.

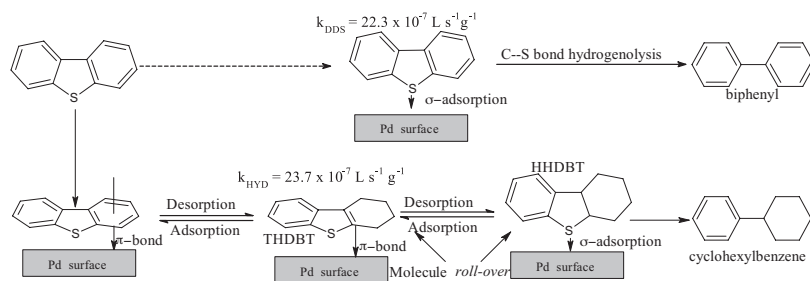


**V.G. Baldovino-Medrano, Sonia A. Giraldo, Aristóbulo Centeno**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 127

Reactivity of dibenzothiophene type molecules over Pd catalysts

The reactivity of DBT type molecules over Pd under HDT conditions was analyzed. High selectivity to the HYD route was interpreted considering Pd interaction with aromatic rings. A mechanism for conversion via HYD comprising saturation of one of the aromatic rings of DBT and roll-over of the molecule onto Pd surface was proposed. Catalytic trends were found to agree well with the characteristics of a Pd metallic active phase.

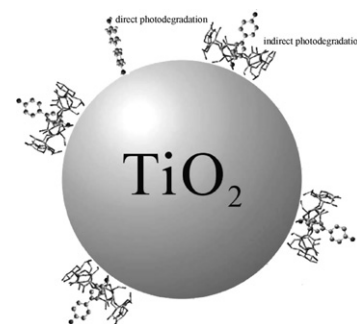


**Xu Zhang, Feng Wu, Zhiping Wang, Yu Guo, Nansheng Deng**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 134

Photocatalytic degradation of 4,4'-biphenol in  $TiO_2$  suspension in the presence of cyclodextrins: A trinity integrated mechanism

A trinity interaction model of 4,4'-biphenol photodegradation in  $TiO_2$  suspension containing cyclodextrin was proposed in this work. Both direct and indirect degradation should be taken into account. It would be beneficial to have a depth-in mechanism of CD effect on reactant's photodegradation in  $TiO_2$  suspension that would probably lead to a high efficiency and selectivity for the photodegradation of pollutants.

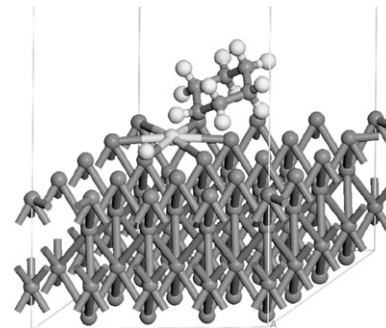


**Pei-Qing Yuan, Bing-Qiang Wang, Yue-Ming Ma, Hui-Min He, Zhen-Min Cheng, Wei-Kang Yuan**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 140

Hydrogenation of cyclohexene over Ru–Zn/Ru(0001) surface alloy: A first principles density functional study

The hydrogenation of cyclohexene over Ru–Zn/Ru(0001) surface alloy was investigated by a DFT study. Both the chemisorption and hydrogenation kinetics of cyclohexene on the surface alloy were found to be depressed, which is supposed to be crucial to the improvement of cyclohexene yield in the partial hydrogenation of benzene over Ru–Zn alloy catalyst.



**Praveen K. Tandon, Mamta Dhusia, Sumita Sahgal**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 146

Oxidation of cyclic ketones by alkaline hexacyanoferrate(III) catalyzed by rhodium(III)

In the oxidation of cyclic ketones by alkaline hexacyanoferrate(III) catalyzed by rhodium(III) rate decreases after a fixed catalyst concentration due to transformation of reactive species of catalyst into the un-reactive one at lower pH of the medium. Hexacyanoferrate(III) is reduced before the slow step with dicarboxylic acid as the oxidation products. Final rate law may be given as-

$$\text{Rate} = \frac{k' [\text{Fey}][\text{S}]_T[\text{OH}][\text{Rh}^{\text{III}}]}{[\text{Feoy}][\text{H}_2\text{O}] + K'[\text{OH}][\text{Fey}]}$$

where-

$$k' = kK_1K_2K_3; K' = K_1K_2$$

$$[\text{Fey}] = [\text{Fe}(\text{CN})_6^{3-}]$$

$$[\text{Feoy}] = [\text{Fe}(\text{CN})_6^{4-}]$$

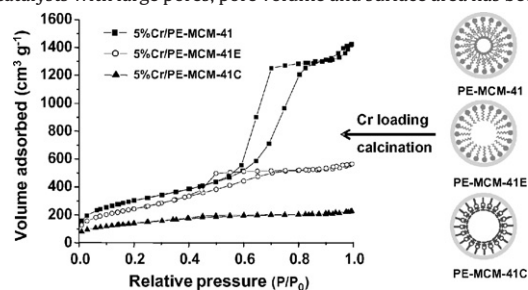
$$[\text{S}]_T = [\text{cyclic ketone}]_{\text{Total}}$$

**T.V. Malleswara Rao, Yong Yang, Abdelhamid Sayari**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 152

Ethane dehydrogenation over pore-expanded mesoporous silica supported chromium oxide: 1. Catalysts preparation and characterization

Pore-expanded MCM-41 silica was prepared hydrothermal treatment of as-synthesized MCM-41 in the presence of dimethyldodecylamine (DMDA). The as-synthesized material (PE-MCM-41), the DMDA-free (PE-MCM-41E) and the organic-free material (PE-MCM-41C) were used as supports for chromium oxide. The structural properties of the materials were associated with the effect of water during impregnation. A general procedure for the preparation of supported catalysts with large pores, pore volume and surface area has been established.



**T.V. Malleswara Rao, El Mamoune Zahidi, Abdelhamid Sayari**

*Journal of Molecular Catalysis A: Chemical* 301 (2009) 159

Ethane dehydrogenation over pore-expanded mesoporous silica-supported chromium oxide: 2. Catalytic properties and nature of active sites

Pore-expanded mesoporous MCM-41 silica-supported chromium oxide materials were found to be very active and highly stable catalysts for ethane dehydrogenation. They were also very selective toward ethylene. Correlation of the reaction rate with *in situ* X-ray photoelectron spectroscopy measurements showed clearly that the Cr(III) species are the main active sites.

