

## Contents

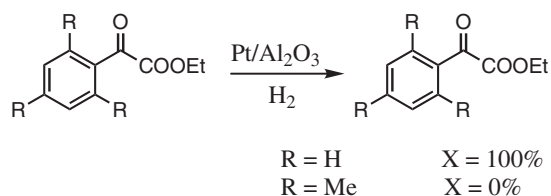
### Articles

**A. Vargas, S. Reimann, S. Diezi, T. Mallat, A. Baiker**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 1

Adsorption modes of aromatic ketones on platinum and their reactivity towards hydrogenation

Hydrogenation of aromatic  $\alpha$ -ketoesters on Pt/Al<sub>2</sub>O<sub>3</sub> under mild conditions showed that ethyl benzoylformate was smoothly hydrogenated, but insertion of two aryl substituents in *o*-position (mesitylglyoxylate and anthracenylglyoxylate) completely eliminated the reactivity of the ketone. Theoretical calculations revealed that *o*-substitution constitutes an impediment to the formation of adsorbed intermediates having the keto-carbonyl group bound to the metal in  $\eta^2$  (C,O) mode.

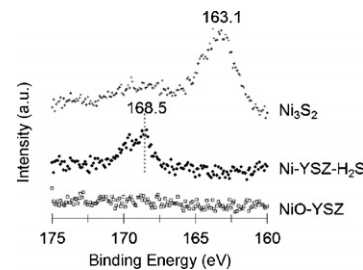


**John N. Kuhn, Nandita Lakshminarayanan, Umit S. Ozkan**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 9

Effect of hydrogen sulfide on the catalytic activity of Ni-YSZ cermets

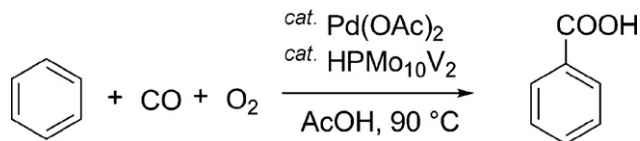
The effect of H<sub>2</sub>S upon the activity and stability of Ni-YSZ (yttria-stabilized zirconia) cermets was examined for model anode chamber reactions. Reactions with H<sub>2</sub>O (water-gas shift reaction, steam reforming) were more strongly affected by sulfur compared to CO or CH<sub>4</sub> oxidation reactions. For reactions involving CH<sub>4</sub>, hydrocarbon decomposition was the dominant reaction pathway at higher temperatures; however, this reaction path was inhibited by sulfur exposure.



**Shingo Yamada, Shin-ichiro Ohashi, Yasushi Obora, Satoshi Sakaguchi, Yasutaka Ishii**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 22

Carboxylation of benzene with CO and O<sub>2</sub> catalyzed by Pd(OAc)<sub>2</sub> combined with molybdovanadophosphates

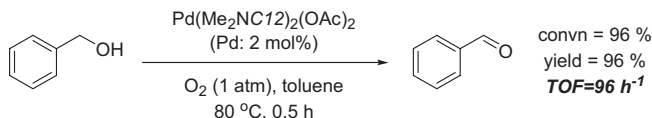


**Shogo Shimazu, Tae Uehara, Aki Asami,  
Takayoshi Hara, Nobuyuki Ichikuni**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 28

Highly efficient alcohol oxidation catalyzed by palladium(II)-alkylamine complexes using atmospheric molecular oxygen

Two series of palladium(II)-alkylamine  $\text{Pd}(\text{Me}_2\text{NCn})_2(\text{OAc})_2$ ,  $\text{Me}_2\text{NCn}$ : *N,N'*-dimethylalkylamine,  $n = 4, 8, 12$ , and 16) and palladium(II)-*N,N'*-dialkylamine  $\text{Pd}(\text{Cn}_2\text{NH})_2(\text{OAc})_2$ ,  $\text{Cn}_2\text{NH}$ : *N,N'*-dialkylamine,  $n = 4, 8$ , and 12) were prepared. These homogeneous Pd complexes catalyzed the aerobic oxidation efficiently, for example, a benzylalcohol oxidation proceeded rapidly by means of  $\text{Pd}(\text{Me}_2\text{NC12})_2(\text{OAc})_2$  with an excellent turnover frequency of as high as  $96 \text{ h}^{-1}$ .

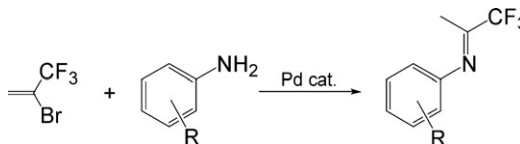


**Tatsuhito Kino, Yu Nagase, Yoshikazu Horino,  
Tetsu Yamakawa**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 34

Pd-catalyzed coupling of arylamines and 2-bromo-3,3,3-trifluoropropene

Pd-catalyzed amination of 2-bromo-3,3,3-trifluoropropene with arylamines to provide (1,1,1-trifluoro-2-propylidene)amine was achieved. By use of 2-aminobenzonitriles and 2-bromoanilines, 4-amino-2-trifluoromethylquinolines and 2-trifluoromethylindoles were obtained, respectively. 1,1,1-trifluoro-2-propylidene group was readily hydrogenated to 1,1,1-trifluoro-2-propyl group by  $\text{LiAlH}_4$ , etc.

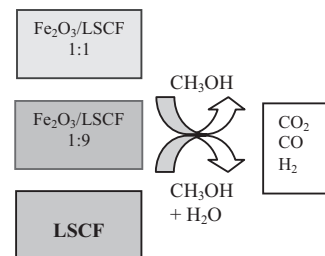


**Alessandro Galenda, Marta Maria Natile,  
Antonella Glisenti**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 52

LSCF and  $\text{Fe}_2\text{O}_3/\text{LSCF}$  powders: Interaction with methanol

This work focalizes on a  $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\delta}$  (LSCF) perovskite and  $\text{Fe}_2\text{O}_3/\text{LSCF}$  nanocomposites. LSCF perovskite is obtained by Pechini method and treated at 1173 K; nanocomposite  $\text{Fe}_2\text{O}_3/\text{LSCF}$  powder samples ( $\text{Fe}_2\text{O}_3/\text{LSCF} = 1:9$  and 1:1 wt.) are obtained by wet impregnation. The reactivity of the obtained samples with respect to pure methanol and to a 1 M aqueous solution of methanol, is investigated.

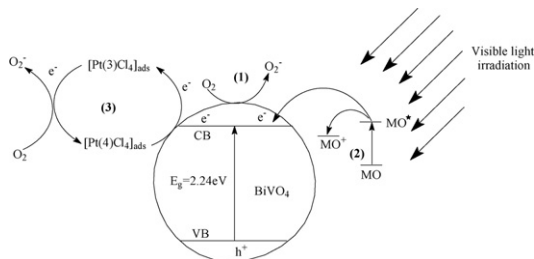


**Lei Ge**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 62

Novel visible-light-driven  $\text{Pt}/\text{BiVO}_4$  photocatalyst for efficient degradation of methyl orange

Visible-light-induced  $\text{Pt}/\text{BiVO}_4$  composite photocatalyst has been synthesized by the impregnation method. The results indicate that the Pt element is present as  $\text{PtCl}_4$  and disperses in the composite samples. The photocatalytic results indicate that the photocatalytic efficiency is significantly improved after the Pt species was loaded. On the basis of experimental results, the platinum chloride can be excited in the visible light region and affords efficient charge transfer in the composite samples.

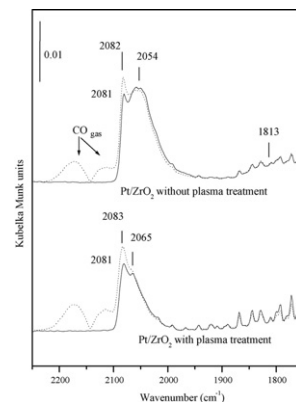


**Xinli Zhu, Yongbing Xie, Chang-jun Liu, Yue-ping Zhang**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 67

Stability of Pt particles on ZrO<sub>2</sub> support during partial oxidation of methane: DRIFT studies of adsorbed CO

DRIFT spectra of adsorbed CO show that Pt sintering is accelerated with increasing calcination temperature. Pt/ZrO<sub>2</sub> deactivation during partial oxidation of methane is not related to coke formation, but to Pt sintering in the presence of oxygen through the Ostwald ripening pathway. Improved resistance to sintering will lead to better stability.

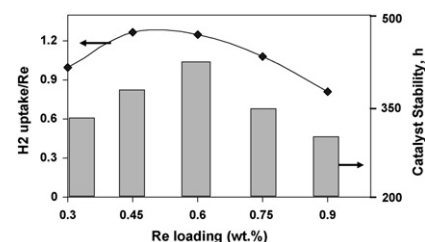


**N. Viswanadham, Raviraj Kamble, Amit Sharma, Manoj Kumar, A.K. Saxena**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 74

Effect of Re on product yields and deactivation patterns of naphtha reforming catalyst

Rhenium loading up to 0.6 wt.% (Re/Pt = 2) facilitated the improvement in hydrogen uptake and hours-on-oil stability of the Pt-Re/Al<sub>2</sub>O<sub>3</sub> naphtha reforming catalyst, while above the 0.6 wt.% loading, the hydrogen uptake as well as catalyst stability is decreased.

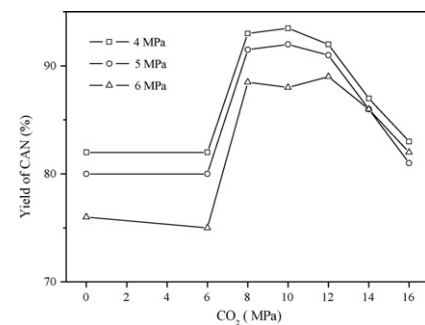


**Chunyu Xi, Haiyang Cheng, Jianmin Hao, Shuxia Cai, Fengyu Zhao**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 80

Hydrogenation of *o*-chloronitrobenzene to *o*-chloroaniline over Pd/C in supercritical carbon dioxide

In the hydrogenation of *o*-CNB over Pd/C, the presence of sCO<sub>2</sub> could improve the yield of *o*-CAN. The reactive rate and the selectivity to *o*-CAN depended largely on CO<sub>2</sub> pressure. In addition, the larger Pd particle benefited the formation of *o*-CAN in sCO<sub>2</sub>.

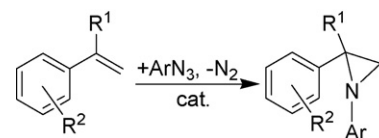


**Emma Gallo, Maria Giovanna Buonomenna, Luca Viganò, Fabio Ragaini, Alessandro Caselli, Simone Fantauzzi, Sergio Cenini, Enrico Drioli**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 85

Heterogenization of ruthenium porphyrin complexes in polymeric membranes: Catalytic aziridination of styrenes

The paper describes the preparation of catalytic membranes having the complex Ru(4-(CF<sub>3</sub>)TPP)CO (1) (TPP = dianion of tetraphenylporphyrin) embedded in the perfluorinated polymer Hyflon AD60X and their use in the aziridination reaction of olefins by aryl azides.



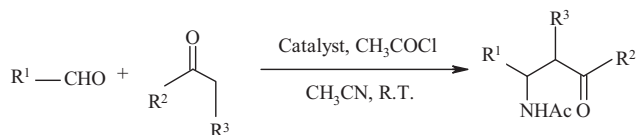
cat. = Ru(4-(CF<sub>3</sub>)TPP)CO-Hyflon AD60X

**E. Rafiee, F. Paknezhad, Sh. Shahebrahimi, M. Joshaghani, S. Eavani, S. Rashidzadeh**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 92

Acid catalysis of different supported heteropoly acids for a one-pot synthesis of  $\beta$ -acetamido ketones

Efficacies of different supported heteropoly acids are investigated for the synthesis of  $\beta$ -acetamido ketones. Various heteropoly acids, catalyst concentration, and heteropoly acids loading on different supports are investigated. Reusability of all supported catalyst is examined. This method consistently has the advantages of excellent yields, short reaction times, and mild reaction conditions. The catalysts are inexpensive, reusable, and ecofriendly solid acids.

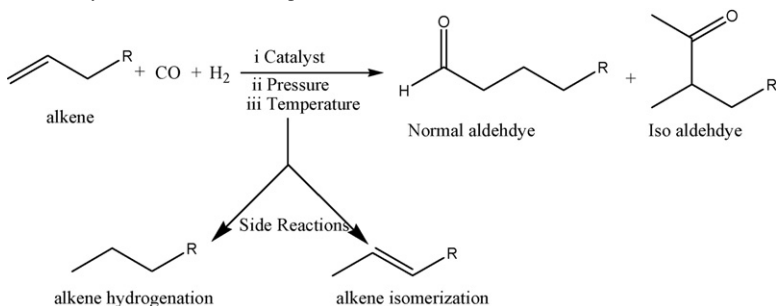


**Asif A. Dabbawala, Dharmesh U. Parmar, Hari C. Bajaj, Raksh V. Jasra**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 99

$\text{CoCl}_2(\text{TPPTS})_2$  catalyzed hydroformylation of 1-octene and 1-decene in the presence of surfactant and co-solvents in a biphasic medium

$\text{CoCl}_2(\text{TPPTS})_2$  catalyzed hydroformylation of higher olefins were studied systematically in an aqueous biphasic system. At optimal condition and with the addition of cationic surfactant, cetyltrimethylammonium bromide (CTAB) hydroformylation reaction rate is greatly accelerated; both high conversion and excellent aldehyde selectivity were obtained in the presence of CTAB.

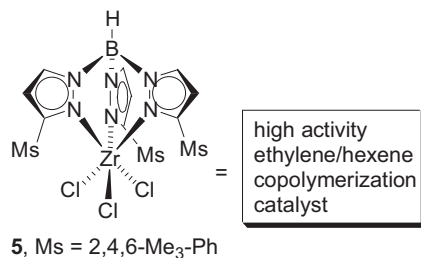


**Kenji Michiue, Richard F. Jordan**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 107

Comparison of olefin polymerization behavior of sterically crowded tris(pyrazolyl)borate group 4 metal complexes

The olefin polymerization performance of sterically crowded group 4 (tris-pyrazolylborate) $\text{MX}_3$ /dried-MAO catalysts was investigated. Diverse behavior is observed for complexes with different metals, oxidation states and ligands.  $\text{Tp}^{\text{Ms}}\text{ZrCl}_3$  (**5**,  $\text{Tp}^{\text{Ms}} = \text{HB}(3\text{-mesitylpyrazolyl})_3^-$ ) produces moderately alternating ethylene/1-hexene copolymer (41 mol% hexene) with ultra-high molecular weight ( $M_w = 1.3 \times 10^6$ ,  $M_w/M_n = 2.2$ ), and uniform composition distribution with high efficiency at 80 °C in toluene.

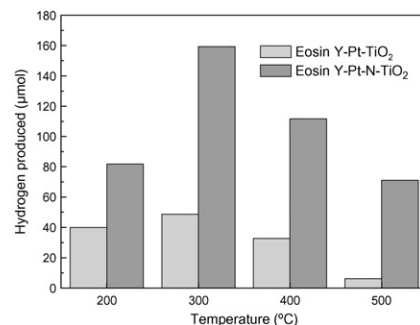


**Yuexiang Li, Chengfu Xie, Shaoqin Peng, Gongxuan Lu, Shuben Li**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 117

Eosin Y-sensitized nitrogen-doped  $\text{TiO}_2$  for efficient visible light photocatalytic hydrogen evolution

The Eosin Y-sensitized platinumized nitrogen-doped  $\text{TiO}_2$  photocatalyst with high visible light activity was prepared. The sensitization of Eosin Y extends the visible light response range of  $\text{N-TiO}_2$ . The  $\text{N-TiO}_2$  has smaller crystalline size and larger specific surface area to enhance the adsorption amount of Eosin Y than  $\text{TiO}_2$  prepared by NaOH. In particular, the surface oxygen defects produced by nitrogen doping would improve adsorption of Eosin Y at the catalyst and excited electron to transfer to the conduction band of  $\text{N-TiO}_2$ . Therefore the photocatalytic activity of Eosin Y-Pt-N- $\text{TiO}_2$  is much higher than that of Eosin Y-Pt- $\text{TiO}_2$ . On the optimum conditions, the activity of Eosin Y-Pt-N- $\text{TiO}_2$ -300 °C is enhanced by a factor 3 compared to that of Eosin Y-Pt- $\text{TiO}_2$ -300 °C.

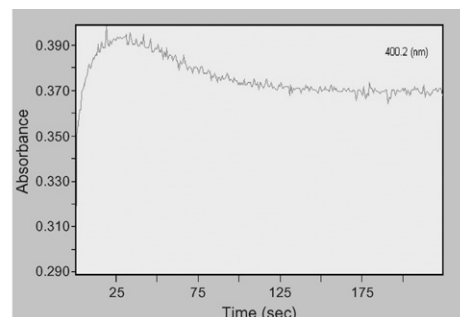
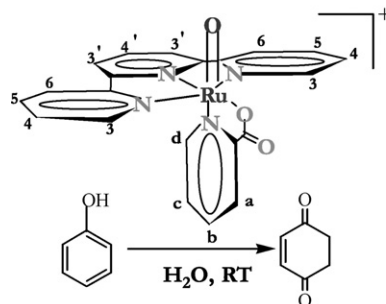


**Debabrata Chatterjee, Anannya Mitra**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 124

Kinetics and catalysis of oxidation of phenol by ruthenium(IV)-oxo complex

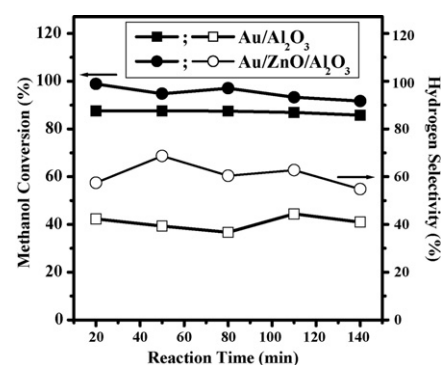
Stopped-flow kinetic studies and SPECFIT global kinetic analysis revealed the presence of two steps in the oxidation of phenol to quinone by  $[\text{Ru}^{\text{IV}}(\text{tpy})(\text{pic})(\text{O})]^+$  in  $\text{H}_2\text{O}$ .

**Feg-Wen Chang, Szu-Chia Lai, L. Selva Roselin**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 129

Hydrogen production by partial oxidation of methanol over ZnO-promoted  $\text{Au}/\text{Al}_2\text{O}_3$  catalysts

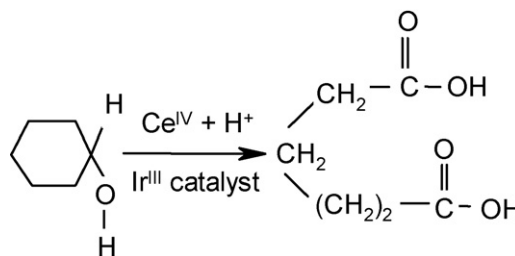
Hydrogen production by partial oxidation of methanol (POM) was investigated over  $\text{Au}/\text{Al}_2\text{O}_3$  and  $\text{Au}/\text{ZnO}/\text{Al}_2\text{O}_3$  catalysts. The  $\text{Au}/\text{ZnO}/\text{Al}_2\text{O}_3$  catalyst showed higher methanol conversion and hydrogen selectivity. The main role of ZnO in promoting the catalytic activity is associated with the progressive formation of smaller Au particles, which are highly dispersed on the surface that comprise active oxygen species for POM.

**Praveen K. Tandon, Alok K. Singh, Sumita Sahgal, Santosh Kumar**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 136

Oxidation of cyclic alcohols by cerium(IV) in acidic medium in the presence of iridium(III) chloride

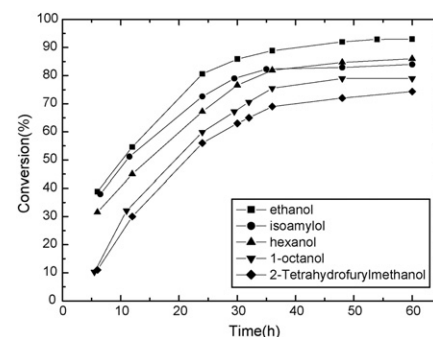
$\text{Ir}^{\text{III}}$  catalyzed oxidation of cyclic alcohols by  $\text{Ce}^{\text{IV}}$  in acidic medium gives dicarboxylic acids.  $\text{Ce}^{\text{III}}$ ,  $\text{Cl}^-$  and  $\text{H}^+$  ions are eliminated before the slow step. Spectral evidence proves that substrate forms complex with cerium and not with catalyst. Catalytic efficiency of iridium(III), surpasses the efficiency of  $\text{Ru}^{\text{III}}$ ,  $\text{Ru}^{\text{VIII}}$  and  $\text{Os}^{\text{VIII}}$ . Cyclooctanol oxidizes easily compared to cyclohexanol.

**Kun Song, Ying Chu, Lihong Dong, Jinling Song, Dan Wang**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 144

Etherification in cyclohexane/DBSA/water microemulsion system

Etherification reaction of hexanol and *tert*-butyl alcohol in the cyclohexane/dodecylbenzenesulfonic acid (DBSA)/water reverse microemulsion system has been investigated. The effect of all kinds of parameters, such as molar ratio of reactants, concentration of DBSA, reaction temperature,  $\omega_0$  value and various substrates, on the etherification was also studied. Furthermore, the comparison reactions in several surfactant systems were also performed and the results showed that the conversion in DBSA system was the highest.

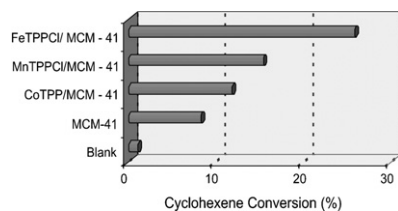


**Andréia A. Costa, Grace F. Ghesti,  
Julio L. de Macedo, Valdeilson S. Braga,  
Marcello M. Santos, José A. Dias, Sílvia C.L. Dias**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 149

Immobilization of Fe, Mn and Co tetraphenylporphyrin complexes in MCM-41 and their catalytic activity in cyclohexene oxidation reaction by hydrogen peroxide

Synthesis, characterization and application of three metalloporphyrin catalysts (FeTPPCL, MnTPPCL and CoTPP), where TPP = tetraphenylporphyrin) anchored on MCM-41, in cyclohexene oxidation with hydrogen peroxide are reported. FeTPPCL/MCM-41 showed higher conversion than CoTPP/MCM-41 and MnTPPCL/MCM-41. MnTPPCL/MCM-41 (which had the lowest concentration) showed the highest turnover number. All catalysts exhibited similar selectivity that favors allylic oxidation products over epoxidation.



**Gina Pecchi, Claudia Campos, Octavio Peña,  
Luis E. Cadus**

*Journal of Molecular Catalysis A: Chemical* 282 (2008) 158

Structural, magnetic and catalytic properties of perovskite-type mixed oxides  $\text{LaMn}_{1-y}\text{Co}_y\text{O}_3$  ( $y = 0.0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0$ )

Substituted  $\text{LaMn}_{1-y}\text{Co}_y\text{O}_3$  perovskite-type oxides ( $0.0 \leq y_{\text{Co}} \leq 1.0$ ) have been investigated as catalysts in the total combustion of acetylacetate. The characterization indicates variation in specific surface area, crystal structure and reducibility. The crystal phase transformation occurs for  $y_{\text{Co}} > 0.5$ , and the role of Mn is to stabilize the cobaltite structure, which does not tolerate more than 30% substitution.

