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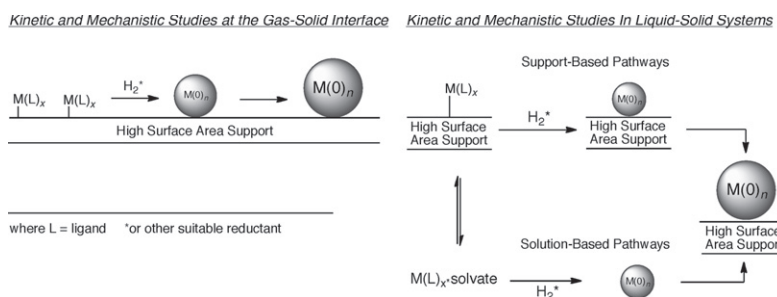
Articles

**Joseph E. Mondloch, Ercan Bayram,
Richard G. Finke**

Journal of Molecular Catalysis A: Chemical 355 (2012) 1

A review of the kinetics and mechanisms of formation of supported-nanoparticle heterogeneous catalysts

► The kinetics and mechanisms of formation of practical, supported-nanoparticle heterogeneous catalysts have been reviewed. ► The extant literature contains 39 kinetic and mechanistic studies in the gas–solid interface, but only 8 kinetic and mechanistic studies in the lesser investigated liquid–solid systems. ► The insights herein should provide guidance to the synthesis of better size, shape and compositionally controlled supported-nanoparticle catalysts.

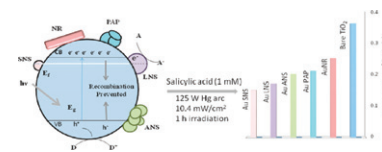


Rupinder Kaur, Bonamali Pal

Journal of Molecular Catalysis A: Chemical 355 (2012) 39

Size and shape dependent attachments of Au nanostructures to TiO₂ for optimum reactivity of Au–TiO₂ photocatalysis

► TiO₂ photoactivity improved with decreasing size (9.5 > 3.5 nm) of Au co-catalysts. ► Au nanosphere (3.5 nm) co-catalytic activity is higher than Au nanorod. ► Au co-catalytic ability reduced with decreasing surface to volume ratio. ► Aggregation of Au nanoparticles lowered the TiO₂ photocatalytic activity. ► Au co-catalysts required (0.02 wt%) for TiO₂ photoactivity is 100 times less.

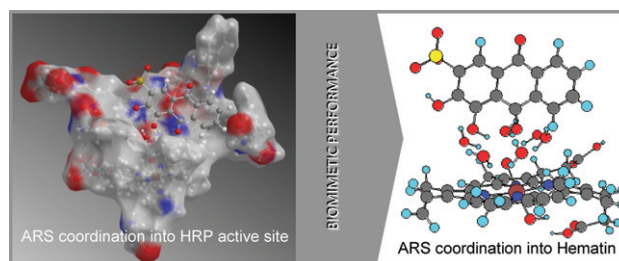


**Agostina Córdoba, Ivana Magario,
María Luján Ferreira**

Journal of Molecular Catalysis A: Chemical 355 (2012) 44

Experimental design and MM2–PM6 molecular modelling of hematin as a peroxidase-like catalyst in Alizarin Red S degradation

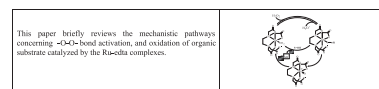
► Hematin emerges as an efficient catalyst for ARS decolorization. ► Analysis of substrate coordination demonstrates the flexibility of hematin. ► The blocking of HRP active site by bulky substrates was demonstrated. ► The key role of the H₂O coordinated in the HRP Cpd-I mechanism was discussed.



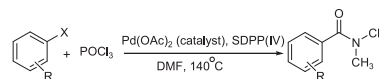
Debabrata Chatterjee, Rudi van Eldik*Journal of Molecular Catalysis A: Chemical* 355 (2012) 61

Mechanism of –O–O–1 bond activation and substrate oxidation by Ru-edta complexes

► –O–O– bond activation by Ru-edta type complexes. ► Catalysis of oxidation of bio-molecules by Ruedta complex-biological significance. ► Catalysis of dye-degradation by Ru-edta type complex – environmental significance. ► Mechanistic knowledge on the catalytic process in terms of –O–O– bond activation.

**Nasser Iranpoor, Habib Firouzabadi, Somayeh Motevali***Journal of Molecular Catalysis A: Chemical* 355 (2012) 69Silicadiphenyl phosphinite (SDPP)/Pd(0) nanocatalyst for efficient aminocarbonylation of aryl halides with POCl₃ and DMF

► Silicaphosphinite and Pd(II) act as an efficient catalyst for the amidation. ► Amides are obtained in high yields from aryl halides by using of POCl₃ and DMF. ► The use of combination of POCl₃ and DMF is as an easy approach for amide synthesis.

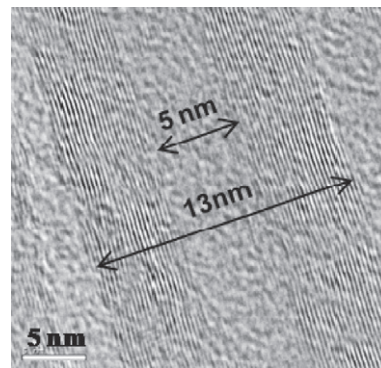


X: I; R: H, NO₂, CN, CH₃, OCH₃, OH
 X: Cl, Br; R: H, NO₂, CN
 SDPP(IV): silicadiphenyl phosphinite

R. Atchudan, A. Pandurangan*Journal of Molecular Catalysis A: Chemical* 355 (2012) 75

The use of bimetallic MCM-41 mesoporous catalysts for the synthesis of MWCNTs by chemical vapor deposition

► Synthesis and characterization of Cr-MCM-41 and metal loaded Cr-MCM-41. ► Synthesis of well-ordered MWCNTs using efficient Fe/Cr-MCM-41 by CVD method. ► The bimetallic MCM-41 is suitable supports for catalytically synthesizing MWCNTs.

**Percy van der Gryp, Sanette Marx, Hermanus C.M. Vosloo***Journal of Molecular Catalysis A: Chemical* 355 (2012) 85

Experimental, DFT and kinetic study of 1-octene metathesis with Hoveyda-Grubbs second generation precatalyst

► Catalytic performances of Hoveyda-Grubbs 2-generation for 1-octene metathesis. ► Present an empirical reaction kinetic model. ► DFT-study of mechanism and comparison.

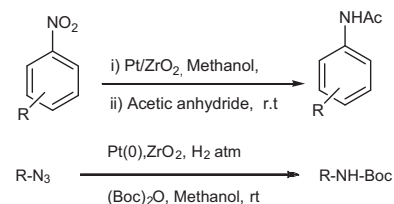


M. Lakshmi Kantam, R. Sudarshan Reddy, K. Srinivas, R. Chakravarti, B. Sreedhar, F. Figueras, Ch. Venkat Reddy

Journal of Molecular Catalysis A: Chemical 355 (2012) 96

Platinum nanoparticles supported on zirconia mediated synthesis of N-acyl and N-(*tert*-butoxycarbonyl)amines from nitroarenes and azides

► One-pot synthesis of carbamates from corresponding nitro and azide compounds. ► Environment friendly methodology, utilizing molecular hydrogen as the reductant. ► Bi-functional Pt(0)/ZrO₂ shows high efficiency in reduction followed by protection. ► Catalyst reused several times without loss of activity. ► Industrially viable reaction smoothly affording good yields under mild conditions.

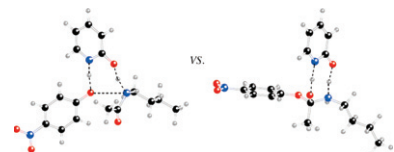


Xiao-Qiang Liu, Lu Jin, Chan Kyung Kim, Ying Xue

Journal of Molecular Catalysis A: Chemical 355 (2012) 102

Role of bifunctional catalyst 2-pyridone in the aminolysis of *p*-nitrophenyl acetate with *n*-butylamine: A computational study

► Three possible mechanisms for the title reaction are considered. ► The stepwise pathway through zwitterionic intermediates is the most favored. ► 2-Pyridone accelerates the reaction with supramolecular effect and proton shuttle.

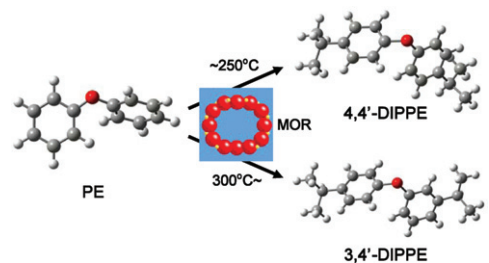


Yoshihiro Sugi, Masateru Kamiya, Hiroshi Tamada, Natsuko Kobayashi, Ikuyo Toyama, Shogo Tawada, Kenichi Komura, Yoshihiro Kubota, Anand Chokkalingam, Ajayan Vinu

Journal of Molecular Catalysis A: Chemical 355 (2012) 113

The isopropylation of diphenyl ether over H-mordenite catalysts

► Shape-selective isopropylation of diphenyl ether (PE) occurred over MOR. ► 4,4'-Diisopropylidiphenyl ether (4,4'-DIPPE) was formed selectively at 175–250 °C. ► 3,4'-DIPPE were predominant isomer with increase in reaction temperature to 300–350 °C. ► 4,4'-DIPPE was isomerized to stable 3,4'-DIPPE at internal and external acid sites. ► Isomerization is due to fluctuation of zeolite channel and flexibility of 4,4'-DIPPE.

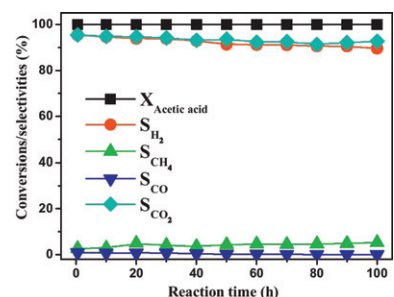


Zhikun Li, Xun Hu, Lijun Zhang, Gongxuan Lu

Journal of Molecular Catalysis A: Chemical 355 (2012) 123

Renewable hydrogen production by a mild-temperature steam reforming of the model compound acetic acid derived from bio-oil

► Low-temperature steam reforming of acetic acid was investigated over Ni-containing catalysts. ► The reaction parameters have quite different effects on the production of hydrogen. ► Ni/La₂O₃ had the highest catalytic activity compared to Ni/ZnO, Ni/CeO₂ and Ni/ZrO₂. ► Methyl species and hydroxyl species played different roles for the formation of the products.

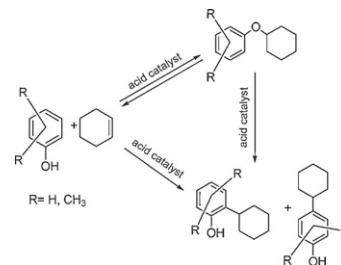


L. Ronchin, A. Vavasori, L. Toniolo

Journal of Molecular Catalysis A: Chemical 355 (2012) 134

Acid catalyzed alkylation of phenols with cyclohexene: Comparison between homogeneous and heterogeneous catalysis, influence of cyclohexyl phenyl ether equilibrium and of the substituent on reaction rate and selectivity

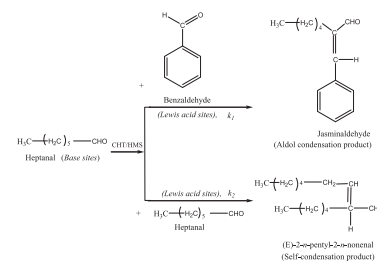
► Cyclohexylation of several phenols in the presence of heterogeneous and homogeneous acid catalysts. ► O-alkylations and ring alkylations always occur, different *ortho/para* ratio occurs by varying the catalysts. ► Cyclohexyl phenyl ether concentration influences the formation of the *ortho*-isomer. ► Formation of cyclohexyl phenyl ether is reversible that of cyclohexylphenols is not. ► Steric hindrance of the substituent influences selectivity more than its inductive effect.

**Ganapati D. Yadav, Pawan kumar Adari**

Journal of Molecular Catalysis A: Chemical 355 (2012) 142

Aldol condensation of benzaldehyde with heptanal to jasminaldehyde over novel Mg–Al mixed oxide on hexagonal mesoporous silica

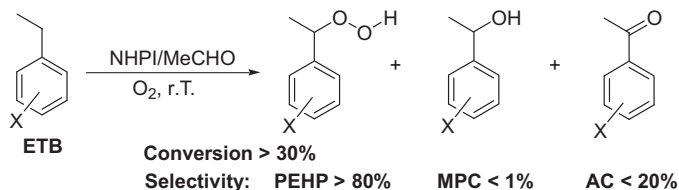
► Novel 20% calcined hydrotalcite supported on hexagonal mesoporous silica. ► Aldol condensation of heptanal with benzaldehyde to jasminaldehyde. ► Heptanal to benzaldehyde mole ratio – 1:5, 150 °C. ► 86% selectivity to jasminaldehyde. ► Mechanism and kinetics of reaction.

**Lucio Melone, Simona Prosperini, Cristian Gambarotti, Nadia Pastori, Francesco Recupero, Carlo Punta**

Journal of Molecular Catalysis A: Chemical 355 (2012) 155

Selective catalytic aerobic oxidation of substituted ethylbenzenes under mild conditions

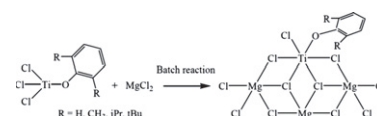
► We have developed a metal-free catalytic system consisting of an aldehyde and NHPI. ► We have employed the catalytic system for the oxidation of substituted ethylbenzenes. ► We have shown the high selectivity in the hydroperoxide products. ► We have shown the marked polar effect in the presence of the catalytic system. ► We have studied the effect of temperature and catalyst and substrate concentration.

**Shengjie Xia, Zhisheng Fu, Biao Huang, Junting Xu, Zhiqiang Fan**

Journal of Molecular Catalysis A: Chemical 355 (2012) 161

Ethylene/1-hexene copolymerization with MgCl₂-supported Ziegler–Natta catalysts containing aryloxy ligands. Part I: Catalysts prepared by immobilizing TiCl₃(OAr) onto MgCl₂ in batch reaction

► Aryloxy-containing MgCl₂-supported Ziegler–Natta catalysts were prepared. ► The aryloxy/Ti molar ratio in these catalysts were less than 1. ► Different cocatalyst brought about different catalytic behaviors. ► Activated by TIBA, these catalysts produced copolymer with more uniform CCD.

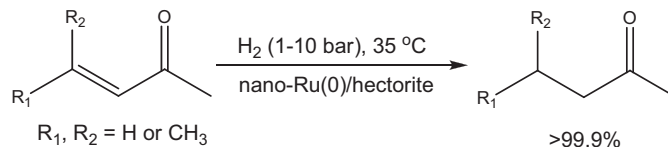


**Farooq-Ahmad Khan, Armelle Vallat,
Georg Süss-Fink**

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Highly selective C=C bond hydrogenation in α,β -unsaturated ketones catalyzed by hectorite-supported ruthenium nanoparticles

► Metallic ruthenium nanoparticles intercalated in hectorite are hydrogenation catalysts. ► They selectively catalyze the C=C bond hydrogenation in α,β -unsaturated ketones. ► The reaction conditions are very mild (35 °C, 1–10 bar H₂ pressure). ► Best results are obtained for selective hydrogenation of mesityl oxide. ► Hectorite-supported ruthenium nanoparticles can be recycled and reused.

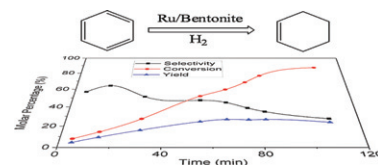


**Weitao Wang, Huizhen Liu, Tianbin Wu,
Peng Zhang, Guodong Ding, Shuguang Liang,
Tao Jiang, Buxing Han**

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Ru catalyst supported on bentonite for partial hydrogenation of benzene to cyclohexene

► Catalysts for selective hydrogenation of benzene to cyclohexene. ► Bentonite, as the low-cost and environmentally friendly support, was employed. ► Ru/bentonite prepared by impregnation-hydrothermal method showed high active. ► Both ZnSO₄ and NaOH significantly improved selectivity. ► Water played an important role in enhancing the selectivity.

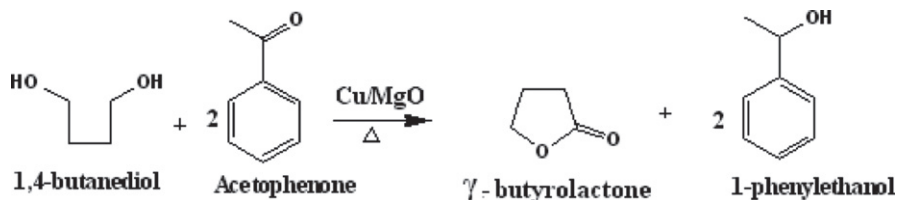


**Kannapu Hari Prasad Reddy, Narani Anand,
Vakati Venkateswarlu,
Kamaraju Seetha Rama Rao, David Raju Burri**

Journal of Molecular Catalysis A: Chemical 355 (2012)
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A selective synthesis of 1-phenylethanol and γ -butyrolactone through coupling processes over Cu/MgO catalysts

► In situ production of hydrogen and its in situ utilization. ► Coupling of 1,4-butanediol dehydrogenation and acetophenone hydrogenation is new. ► Selective production of 1-phenylethanol is a potential application. ► The in situ produced hydrogen need not be purified and stored. ► The overall process is economic, safe and environmentally benign.

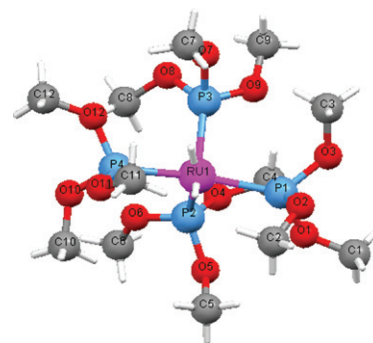


Mehdi Masjedi, Leyla Tatar Yildirim, Saim Özkar

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Novel homogeneous catalyst comprising ruthenium and trimethylphosphite for the hydrolysis of sodium borohydride

► A catalytically active ruthenium(II) species is formed during the hydrolysis of sodium borohydride starting with Ru(acac)₃ and P(OMe)₃. ► A novel ruthenium complex, [Ru{P(OMe)₃}₄H₂], was isolated and fully characterized. ► The active catalyst could be stabilized in the form of [Ru(bipy){P(OMe)₃}(acac)H]. ► The active catalyst is most likely [Ru(acac){P(OMe)₃}₂H], generated by detachment of P(OMe)₃ from the 18-electron fac-[Ru(acac){P(OMe)₃}₃H] complex.

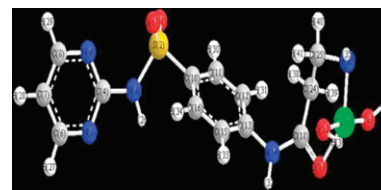


**Ahmed I. Hanafy, Zeinoh M. El-Bahy,
Ahmed A. El-Henawy, Abeer A. Faheim**

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Catalytic oxidation of polyphenol trihydroxybenzene by copper(II) β -alanylsulfadiazine complex

- The ligand has been prepared by reacting sulfadiazine with β alanine amino acid. ► Cu(II) complex of the prepared ligand has been prepared and fully characterized. ► This complex was used as a catalyst for homogenous oxidation of trihydroxybenzene. ► The mechanism of the oxidation was kinetically studied.
- The oxidation has been inhibited by kojic acid.

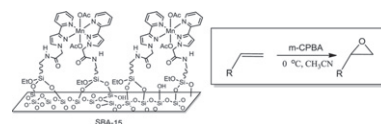


**Jianyuan Tang, Yanhong Zu, Weitao Huo,
Lei Wang, Jing Wang, Mingjun Jia,
Wenxiang Zhang, Werner R. Thiel**

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Mesoporous SBA-15 modified with manganese pyrazolylpyridine complexes for the catalytic epoxidation of terminal alkenes

- Manganese pyrazolylpyridine complexes modified SBA-15 (**5**) is prepared. ► **5** is active and stable heterogeneous catalyst for the epoxidation of terminal alkenes. ► O=Mn^{IV}-species should be the main active intermediates for the epoxidation reaction.

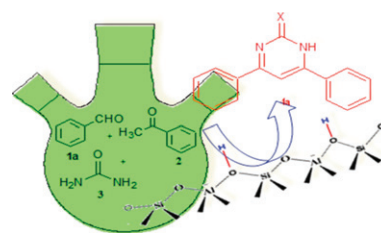


Sunil R. Mistry, Kalpana C. Maheria

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Synthesis of diarylpyrimidinones (DAPMs) using large pore zeolites

- MCRs of biological active DAPM over various large pore zeolites have been studied. ► Focus on elimination of an expensive reagent TMSCl, using large pore zeolites. ► Discussion on plausible mechanism of DAPM synthesis over zeolite.



Mir Ghasem Hosseini, Mohamad Mohsen Momeni

Journal of Molecular Catalysis A: Chemical 355 (2012)
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Fabrication and photo-electrocatalytic activity of highly oriented titania nanotube loaded with platinum nanoparticles for electro-oxidation of lactose: A new recyclable electro-catalyst

- Pt/TNT/Ti catalysts with high porous structure and excellent electro-catalytic were prepared. ► Pt/TNT/Ti showed a remarkably enhanced performance for lactose oxidation under UV lighting. ► Advantages of Pt/TNT/Ti for lactose oxidation are high current density and good stability. ► Anti-poisoning ability of TiO₂ makes Pt/TNT/Ti catalyst reusable after a short UV treatment. ► This study provides a new route for the simple, facile and cost-effective synthesis of Pt/TNT/Ti.

