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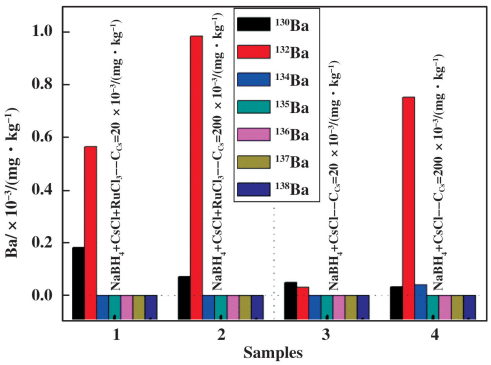
Cs to Ba Element Transmutation in the Presence of Hydride

LU Gong-xuan, ZHANG Xu-qiang

J. Mol. Catal.(China) **2019**, 33(6): 495~500

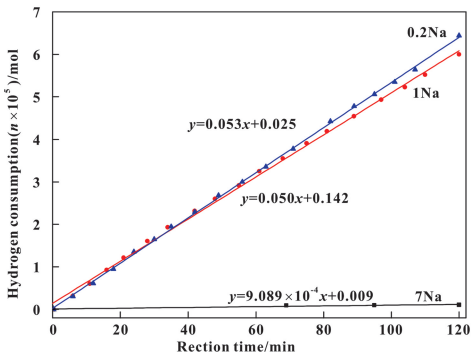


This work reported evidences of Cs to Ba transmutation in the presence of hydride compounds. Experiments identified that the concentration and isotope ratio were changed after reaction of Cs salt with hydride at room temperature. In addition, we confirmed that these phenomena are closely related to Ru catalyst role. Those results imply that some of barium isotope in nature might originate from an unknown low-energy nuclear reaction between Cs and hydride under very mild conditions.

Effect of Residual Na on the Hydrogenation Performance of Nickel Catalysts

GU Ting-ting, ZHAO Hua-hua, YANG Jian, SONG Huan-ling, HAO Yun-qing, CHOU Ling-jun

J. Mol. Catal.(China) **2019**, 33(6): 501~507

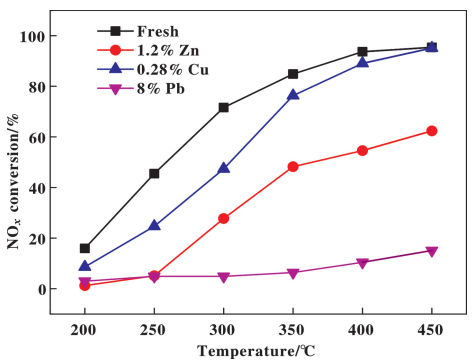


The Ni-Mg/SiO_2 catalysts with the different residual Na contents were prepared by co-precipitation method. These Ni-based catalysts were used for soybean oil hydrogenation, and characterized by ICP-AES, XRD, H_2-TPR, TG-DSC, SEM, and BET. The results show that the activity of hydrogenation to soybean increased with the drop of sodium exsited in nickel catalyst.

Commercial V_2O_5-WO_3/TiO_2 Catalysts for Heavy Metal (Pb, Cu, Zn) Poisoning Mechanism

WANG Dian-er, LI Guo-bo, LI Chao, XU Xin, WANG Ling, ZHANG Ya-ping

J. Mol. Catal.(China) **2019**, 33(6): 508~523

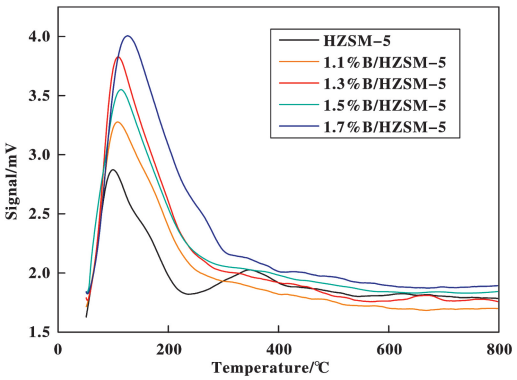


The deNO$_x$ activity of heavy metals (Pb, Cu and Zn) poisoned commercial V_2O_5-WO_3/TiO_2 catalysts prepared by impregnation method showed different degrees of reduction. The characterization results revealed that the deactivation was caused by the coupling effect of chemical and physical poisoning. Due to the relatively high Pb in the simulated heavy metals poisoned catalyst, the deNO$_x$ activity of the Pb poisoned catalysts were reduced obviously, compared to the Cu and Zn poisoned catalyst. Comparing with the fresh commercial V_2O_5/WO_3-TiO_2 catalyst, the addition of Pb, Cu and Zn decreased the BET surface area and total pore volume, changed the pore size distribution of V_2O_5-WO_3/TiO_2 catalyst by blocking its micropore and mesopore, and the BET of the heavy metals poisoned catalysts decreased slowly with the increasing heavy metals contents. The diffraction peak of TiO_2 still existed as anatase crystal, the same as fresh catalyst, and the crystallinity and dispersibility of SCR catalyst was not changed. The presence of Pb, Cu and Zn would reduce the strength of Brønsted and Lewis acids on the catalysts surface, especially the Brønsted acid, which eventually weaken the ability of NH_3 adsorption and activation. The adsorption peak intensity of the adsorbed NO_2 on the heavy metals poisoned catalysts surface, especially the adsorption in the middle and high temperature, the trend of which is more obviously with the increasing heavy metal contents, and the important thing is that increasing NO_2 may promote the formation of N_2O.

The Effect of Boron on HZSM-5 Zeolite Acidity and Shape Selectivity

WU Chao, JI Dong, DONG Peng, LI Hong-wei, LI Gui-xian

J. Mol. Catal.(China) **2019**, 33(6): 524~530



The two peaks of NH_3-TPD desorption for the investigated catalysts, corresponding to weaker acidic (−100 ℃) and stronger acidic sites (−350 ℃) respectively, were demonstrated in above graph. The B/HZSM-5 had almost no strong acid but more weak acid amount than HZSM-5. These acidity variations reflected that the boron modification caused the boron atom to occupy the Brønsted sites and to form a new weak acidity. Para-xylene isomerization was inhibited over weak acidity of B/HZSM-5. Therefore, B/HZSM-5 catalysts exhibited a high p-xylene selectivity over 90%.

Preparation of Ni-Co-Al Mixed Oxides and Their Catalytic Performance for Oxidative Dehydrogenation of Propane

GAO Xiao-xia, WANG Jiang, XU Ai-ju, JIA Mei-lin

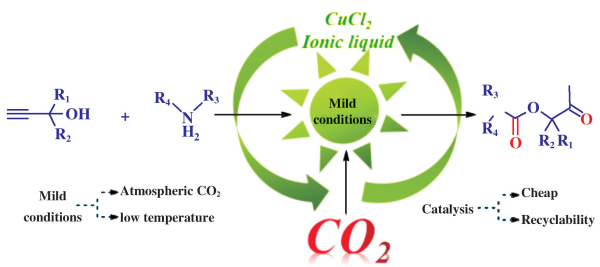
J. Mol. Catal.(China) **2019**, 33(6): 531~541

A series of $3(Ni_xCo_{1-x})Al$ mixed oxide (MMO) catalysts for oxidative dehydrogenation of propane (ODHP) have been derived from $3(Ni_xCo_{1-x})$-Al layered double hydroxide (LDH) precursors (x=1, 0.95, 0.90, 0.75, 0.50, 0.25, 0). $3(Ni_{0.90}Co_{0.10})Al$ MMO had the best catalytic performance: The propylene selectivity was not decreased obviously with the increase of reaction temperature; the propylene yield of 15% at 500 ℃ were observed at the propane conversion of 31%, which is superior to the previously reported MMO catalysts containing Ni or Co. Because there was an electronic interaction between the surface Ni(II) and Co(II/III), the dispersion of the surface NiO-like phase was improved and the surface lattice oxygen species were increased after a small amount of Co doping.

Three-component Reactions of Propargyl Alcohols, Secondary Amines and CO_2 Catalyzed by $CuCl_2$/ Ionic Liquids

LI Di, DU Min-chen, BU Chao, CHEN Cheng, HU Jia, ZHANG Yong-xing, YUAN Ye, Francis Verpoort

J. Mol. Catal.(China) **2019**, 33(6): 542~550

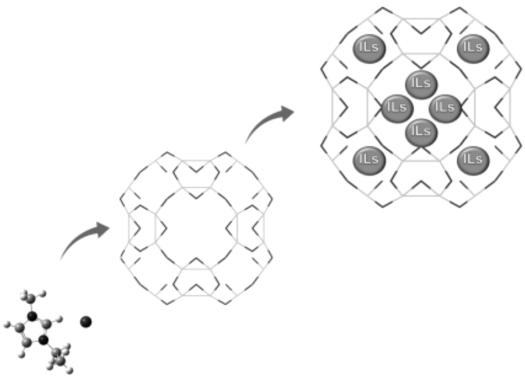


A recyclable and inexpensive $CuCl_2$/ ionic liquid was realized for the synthesis of β-oxopropylcarbamates, transforming a variety of different propargyl alcohols and secondary amines into the target compounds with lower Cu (Ⅱ) loading (2%) under the mild conditions. In addition, this catalytic system could be recycled at least three times without the significant loss of the activity.

DFT Investigation on the CO_2 Adsorption of Confined Ionic Liquids

SUN Yi-fan , JIA Guang-xin, HE Bei-bei

J. Mol. Catal.(China) **2019**, 33(6): 551~560

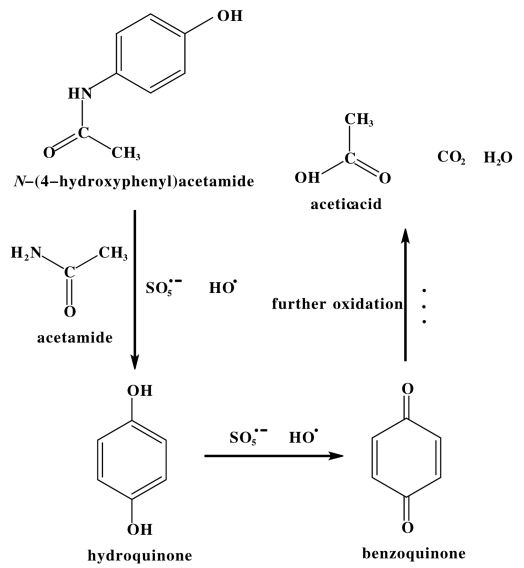


The DFT method is used to study the adsorption of CO_2 by hydrophilic and hydrophobic ionic liquids at different positions. After that, the adsorption of CO_2 by ionic liquids in free state and limited environment was studied. Finding the proper ionic liquids and load positions by comparing the changes in the interaction between CO_2 and the ionic liquids in different environments, finally verifying the above through charge analysis.

Degradation of Acetaminophen in Water by Molecular Sieve Catalyst-Sulfite System

QUAN Xiao-qi, XU Pei-yao, YANG Fan, XIE Wen-fei, WANG Li-dong

J. Mol. Catal.(China) **2019**, 33(6): 561~569



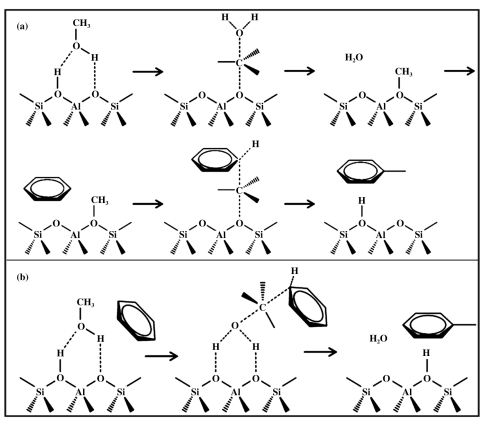
APAP is one of the most common antipyretic and analgesic drugs in medicine, most of which will be metabolized in the liver after entering the body, and the intermediate metabolites can cause toxic and side effects in the liver, kidney, blood system and nervoussystem. Therefore, the management and control of pharmaceutical wastewater containing acetaminophen has attracted extensive attention in recent years.

This paper is based on the fact that cobalt ions activate sulfite at room temperature to produce highly oxidized sulfate radicals($SO_5^{\cdot-}$, $SO_4^{\cdot-}$ and HO ·) to oxidize trace APAP in water. The hydroxyl radical and $SO_5^{\cdot-}$ was first produced, attacks the APAP molecule. Aacetamidecation, which is stripped off and APAP transferred to hydroquinone. Hydroquinone is easily oxidized to p-benzoquinone in the presence of $SO_5^{\cdot-}$. Subsquently, $SO_5^{\cdot-}$ began to attack the C−C and C=C of the p-benzoquinone, leading to the opening of the ring and further formation of inorganic small molecules(CH_3COOH), CO_2 and H_2O More importantly, the Co^{2+} are loaded on SBA-15 mesoporous zeolite by dipping method, and the heterogeneous catalytic oxidation method is adopted to prevent metal ions from directly dissolving into water and causing secondary pollution to water.

Research Progress of ZSM-5 Molecular Sieve Catalyzing Alkylation of Benzene with Methanol

LI Gui-xian, ZHANG Yong-fu, DONG Peng, GUO Yong-qi

J. Mol. Catal.(China) **2019**, 33(6): 570~577

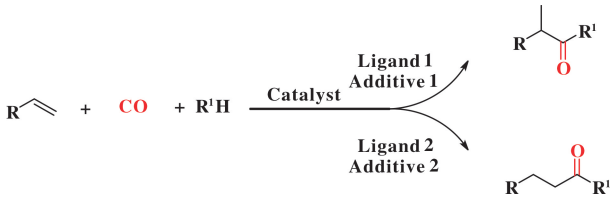


The research progress of ZSM-5 catalysts and mechanism for alkylation of benzene and methanol were detailed. The research direction of benzene alkylation with methanol was summarized and prospected, which provided a reference for the industrial application of the reaction.

Recent Advances on Regioselectivity of Carbonylation Reaction

HUANG Zi-jun, WU Shan-xuan, LI Yue-hui

J. Mol. Catal.(China) **2019**, 33(6): 578~591



Carbonylation reaction is the chemistry process of introducing the carbonyl group (C=O) into the substrates in the presence of catalysts. Carbonylation is an important way to prepare carbonyl compounds, which can provide high added value and high purity carbonyl compounds. Impactful regioselectivity control is crucial for cost-effectivechemical synthesis. This review article overviews development of carbonylation reactions and future trends onregioselectivity for the past few years.

《分子催化》简介

《分子催化》是由中国科学院兰州化学物理研究所主办、中国科学院主管、科学出版社出版的向国内外公开发行的学术性刊物. 主要报道有关分子催化方面最新进展与研究成果. 辟有学术论文、研究简报、研究快报及综合述评等栏目. 内容侧重于配位催化、酶催化、光助催化、催化过程中的立体化学问题、催化反应机理与动力学、催化剂表面态的研究及量子化学在催化学科中的应用等. 工业催化过程中的均相催化剂、固载化学的均相催化剂、固载化的酶催化剂等活化、失活和再生; 用于新催化过程的催化剂的优选与表征等方面的内容, 本刊亦有报道. 读者对象主要是科研单位及工矿企业中从事催化工作的科技人员、研究生、高等院校化学系和化工系的师生.

《分子催化》已被美国化学文摘(CA)、俄罗斯化学文摘、中国科学引文数据库、中国化学文献数据库、中国学术期刊文摘、中国化工文摘等国内外文献数据库收录.《分子催化》现为《中文核心期刊要目总览》的中国核心期刊和中国科技核心期刊. 曾荣获中科院和甘肃省科委“优秀期刊三等奖”和“优秀科技期刊”奖.

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