Exploring the Synthesis of Mesoporous Stannosilicates as Catalysts for the Conversion of Mono- and Oligosaccharides into Methyl Lactate

Sn-Beta zeolites are among the most promising catalysts for the conversion of biomasses due to their high Lewis acidity, which allows coordination to functionalized molecules and promotes cleavage and rearrangement reactions. For applications in biorefining zeolite porosity would ideally be optimized to avoid diffusional limitations, which otherwise may decrease reaction rates and restrict the conversion of bulky substrates. The synthesis of mesoporous zeolites can help alleviating limitations and is a central topic in heterogeneous catalysis, with many synthetic procedures for mesoporous zeolites proposed over the last decades. Here, we explore different syntheses routes to prepare Lewis acidic Sn-containing zeolites, and the main features of the prepared mesoporous materials are characterized. We investigate the correlation between different types of porosity and the activity for the conversion of sugars into methyl lactate. The monomer glucose, the dimer sucrose and the oligomer inulin are applied as model substrates for the reaction in order to probe the accessibility of molecules with different sizes to active sites in zeolites with different pore systems.

General information
State: Accepted/In press
Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, University of Bologna, Haldor Topsoe AS
Contributors: Tosi, I., Sacchetti, A., Martinez-Espin, J. S., Meier, S., Riisager, A.
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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.57 SJR 0.965 SNIP 0.753
Web of Science (2017): Impact factor 2.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.877
Web of Science (2016): Impact factor 2.486
Homogeneously-catalysed hydrogen release/storage using the 2-methylindole/2-methylindoline LOHC system in molten salt-organic biphasic reaction systems

Ir-Complex catalysed hydrogen release/storage using a 2-methylindole/2-methylindoline Liquid Organic Hydrogen Carrier (LOHC) system is shown to be effective in a temperature range of 120 to 140 °C. In the form of a liquid-liquid biphasic reaction system with molten [PPh₄][NTf₂] as catalyst immobilisation phase, the applied cationic Ir-complex can be easily separated and recycled enabling a small amount of ionic catalyst solution to store/release a large amount of hydrogen.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark, Friedrich-Alexander-Universität Erlangen-Nürnberg
Contributors: Søgaard, A., Scheuermeyer, M., Bösmann, A., Wasserscheid, P., Riisager, A.
Number of pages: 4
Pages: 2046-2049
Publication date: 2019
Peer-reviewed: Yes

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Journal: Chemical Communications
Volume: 55
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ISSN (Print): 1359-7345
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127
Web of Science (2017): Impact factor 6.29
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.06 SJR 2.538 SNIP 1.16
Web of Science (2016): Impact factor 6.319
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.7 SJR 2.601 SNIP 1.295
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.83 SJR 2.692 SNIP 1.436
Web of Science (2014): Impact factor 6.834
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.73 SJR 2.752 SNIP 1.372
Web of Science (2013): Impact factor 6.718
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.21 SJR 3.118 SNIP 1.35
Web of Science (2012): Impact factor 6.378
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.96 SJR 2.889 SNIP 1.323
Web of Science (2011): Impact factor 6.169
MnOx/P25 with tuned surface structures of anatase-rutile phase for aerobic oxidation of 5-hydroxymethylfurfural into 2,5-diformylfuran

A series of MnOx/P25 (TiO2) catalysts were prepared by a simple impregnation method and evaluated for the selective oxidation of 5-hydroxymethylfurfural (HMF) into 2,5-diformylfuran (DFF). The as-prepared catalysts were characterized by N2 adsorption/desorption isotherms, transmission electron microscope (TEM), X-ray powder diffraction (XRD), hydrogen temperature-programmed reduction (H2-TPR), Raman, and thermogravimetric analysis. The surface anatase-rutile structure of P25 can be tuned via calcination at different temperature for different time and has significant effects on the catalytic activity of MnOx/P25 for HMF oxidation. The results reveal that MnOx supported on P25 pretreated at 600°C for 5h (MnOx/P25-600-5h) shows the best catalytic performance achieving 33.2% HMF conversion along with 97.0% selectivity to DFF in a two-hour reaction time. The catalytic activity of MnOx/P25-600-5h is almost twice higher than untreated MnOx/P25 catalyst, attributing to the optimized surface structures of anatase/rutile ratio (1.83). In addition, the effects of MnOx loadings, reaction time and temperature of the catalysts for HMF oxidation were also investigation. Furthermore, the MnOx/P25-600-5h catalyst can be used for five consecutive runs without significant loss of its catalytic activity.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, East China University of Science and Technology, Technical University of Denmark
Contributors: Chen, L., Yang, W., Gui, Z., Saravanamurugan, S., Riisager, A., Cao, W., Qi, Z.
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Publication information
Journal: Catalysis Today
Volume: 319
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Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.55 SJR 1.347 SNIP 1.329
Web of Science (2017): Impact factor 4.667
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.322 SNIP 1.369
Web of Science (2016): Impact factor 4.636
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4 SJR 1.335 SNIP 1.403
Web of Science (2015): Impact factor 4.312
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.72 SJR 1.315 SNIP 1.453
Web of Science (2014): Impact factor 3.893
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.39 SJR 1.299 SNIP 1.415
Web of Science (2013): Impact factor 3.309
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.38 SJR 1.469 SNIP 1.422
Web of Science (2012): Impact factor 2.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.34 SJR 1.472 SNIP 1.562
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.761 SNIP 1.449
Web of Science (2010): Impact factor 2.993
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.718 SNIP 1.631
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.692 SNIP 1.533
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.595 SNIP 1.594
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.512 SNIP 1.346
Pd-catalysed formation of ester products from cascade reaction of 5-hydroxymethylfurfural with 1-hexene

A cascade reaction involving decarbonylation of 5-hydroxymethylfurfural (HMF) followed by methoxycarbonylation of 1-hexene produces methyl heptanoate (MH) using a catalytic system composed of a Pd-phosphine complex and methanesulfonic acid (MSA) co-catalyst at moderate reaction temperature. Concomitant hydration of HMF followed by hydrogenation of methyl levulinate (ML) to γ-valerolactone (GVL) occurs with the catalytic system under the same reaction conditions using HMF and methanol as the source of CO and H₂, respectively. Under optimized reaction conditions, about 50% of MH along with 12% ML and 35% GVL is obtained from HMF using Pd-(1,2-bis(di-tert-butylphosphinomethyl)benzene) (DTBPMB), MSA and 1-hexene in methanol at 120 °C. Interestingly, sugars, such as glucose, fructose and xylene, are able to be converted to MH, ML and GVL as well. Isotopic labeling studies with 13C labelled fructose in methanol-d⁴ and 13C-methanol-d⁴ confirm that H₂ originates from methanol, while CO generates predominantly from the formyl group of the HMF formed by fructose dehydration.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Organic Chemistry, Guizhou University
Contributors: Garcia-Suarez, E. J., Paolicchi, D., Li, H., He, J., Yang, S., Riisager, A., Saravanamurugan, S.
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Publication information
Journal: Applied Catalysis A: General
Volume: 569
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Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.48 SJR 1.237 SNIP 1.257
Web of Science (2017): Impact factor 4.521
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.202 SNIP 1.336
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.08 SJR 1.218 SNIP 1.427
Catalytic Tandem Reaction for the Production of Jet and Diesel Fuel Range Alkanes

Jet and diesel fuels are typically composed of $C_9-C_{14}$ and $C_{12}-C_{20}$ hydrocarbons, respectively, but the carbon-chain length of sugar-derived aldehydes and furanic compounds is no longer than $C_6$. Here, a cascade catalytic process involving alkylation and hydrodeoxygenation (HDO) of 2-methylfuran (2-MF) with different aldehydes is conducted to directly produce long-chain alkanes with exclusive carbon number of $C_{11}-C_{17}$ in overall yields of 50-84%. Preliminary investigations on the alkylation of 2-MF and formalin show that the relative density of Lewis and Brønsted acidic sites of zeolitic materials remarkably affect their catalytic activity and selectivity. Sn-beta(12.5) with pronounced Lewis acidity (including the acid density and strength) exhibits higher catalytic performance in the alkylation than other zeolites, producing long-chain oxygenates in 58-92% yields. Even in aqueous solution, the Sn-beta(12.5) catalyst can be reused for at least six reaction cycles with almost constant reactivity. More importantly, the co-addition of Hf(OTf)$_4$ with Pd/C greatly promotes C-O bond cleavage of the furan-ring during the HDO process under mild reaction conditions, producing long-chain alkanes in high yields of 84-94%.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, Guizhou University, East China University of Science and Technology
Contributors: Li, H., Gui, Z., Yang, S., Qi, Z., Saravanamurugan, S., Riisager, A.
Pages: 1060-1066
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Energy Technology
Volume: 6
Issue number: 6
ISSN (Print): 2194-4288
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.83
Web of Science (2017): Impact factor 3.175
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 0.66
Web of Science (2016): Impact factor 2.789
Scopus rating (2015): CiteScore 0.21
Web of Science (2015): Impact factor 2.557
Web of Science (2014): Impact factor 2.824
Original language: English
DOIs:
10.1002/ente.201700637
Source: FindIt
Source-ID: 2392509597
Research output: Research - peer-review » Journal article – Annual report year: 2018

Catalytic Transfer Hydrogenation of Bio-Based Furfural with NiO Nanoparticles

A facile yet highly efficient catalytic system was developed for the catalytic transfer hydrogenation (CTH) of biomass-derived furfural (FF) to furfuryl alcohol (FAOL) over commercially available NiO nanoparticles using 2-propanol as solvent and H-donor. The catalyst system yielded 94.4% of FAOL after only 30 min of reaction at 170 °C, and a satisfactory FAOL yield of 80.9% was also attained under milder reaction conditions (150 °C, 4 h). Furthermore, the NiO catalyst proved reusable for CTH of FF several times maintaining its pristine activity after calcination in air. The catalyst effectiveness was further confirmed by performing scaled-up CTH of FF and CTH of various other aldehydes. Compared to other Ni-based catalysts reported for the hydrogenation of FF, the present system absolutely averted using H2 gas as pure NiO nanoparticles with acid-base properties did not require pre-reduction.

General information
State: Published
Control of selectivity in hydrosilane-promoted heterogeneous palladium-catalysed reduction of furfural and aromatic carboxides

The production of liquid fuels and fine chemicals often involves multi-step reaction processes with selective hydrogenation as one of the key steps. This step most often depends on high-pressure excess hydrogen gas, fossil resources, and newly prepared metallic catalysts. Here we describe an approach to tune activity and selectivity toward transfer hydrogenation of renewable biomass derivatives over commercially available Pd/C using liquid hydrosilane as hydrogen source. The appropriate control of water-doping content, acid type, reaction temperature, and liquid H− donor dosage permits the selective formation of four different value-added products in high yields (≥90%) from bio-based furfural under mild reaction conditions (15–100 °C). Mechanistic insights into the hydrosilane-mediated cascade reactions of furfural are obtained using isotope labeling. The catalyst is recyclable and can selectively reduce an extensive range of aromatic carbonyl compounds to the corresponding alcohols or hydrocarbons in 83–99% yield, typically at 25–40 °C.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry, Guizhou University, Center of Innovative and Applied Bioprocessing, Graduate University of Chinese Academy of Sciences
Fifteen Years of Supported Ionic Liquid Phase-Catalyzed Hydroformylation: Material and Process Developments

This review describes the development of supported ionic liquid phase (SILP) materials as novel hydroformylation catalysts. Ligand-modified rhodium catalysts can be immobilized in a thin film of ionic liquid, which itself is dispersed on a porous material. The solid SILP catalysts have been improved with respect to activity, selectivity, and stability. In addition, their applicability in continuous gas-phase processes opens new opportunities for improved chemical production routes.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Ruhr University Bochum, Friedrich-Alexander-Universität Erlangen-Nürnberg
Contributors: Marinkovic, J. M., Riisager, A., Franke, R., Wasserscheid, P., Haumann, M.
Number of pages: 12
Publication date: 2018
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Journal: Industrial and Engineering Chemistry Research
ISSN (Print): 0888-5885
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
Kinetic Analysis of Hexose Conversion to Methyl Lactate by Sn Beta: Effects of Substrate Masking and of Water

Simple sugars bear promise as substrates for the formation of fuels and chemicals using heterogeneous catalysts in alcoholic solvents. Sn-Beta is a particularly well suited catalyst for the cleavage, isomerization and dehydration of sugars into more valuable chemicals. In order to understand these processes and save resources and time by optimising them, kinetic and mechanistic analyses are helpful. Herein, we study substrate entry into the Sn-Beta catalysed methyl lactate process using abundant hexose substrates. NMR spectroscopy is applied to show that the formation of methyl lactate occurs in two kinetic regimes for fructose, glucose and sucrose. The majority of methyl lactate is not formed from the substrate directly, but from methyl fructosides in a slow regime. At 160 °C, more than 40% of substrate carbon are masked (i.e. reversibly protected in situ) as methyl fructosides within few minutes when using hydrothermally synthesised Sn-Beta, while more than 60% methyl fructosides can be produced within few minutes using post synthetically synthesised Sn-Beta. A significant fraction of substrate thus is masked by rapid methyl fructoside formation prior to subsequent slow release of...
fructose. This release is the rate limiting step in the Sn-Beta catalysed methyl lactate process, but can be accelerated by the addition of small amounts of water at the expense of maximum methyl lactate yield.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Center for Hyperpolarization in Magnetic Resonance, Department of Electrical Engineering, Center for Magnetic Resonance, Haldor Topsoe AS
Contributors: Tosi, I., Riisager, A., Taarning, E., Jensen, P. R., Meier, S.
Number of pages: 9
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**Publication information**

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BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
Web of Science (2017): Impact factor 5.365
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.64 SJR 1.811 SNIP 1.287
Web of Science (2016): Impact factor 5.773
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.46 SJR 1.804 SNIP 1.314
Web of Science (2015): Impact factor 5.287
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.44 SJR 1.885 SNIP 1.47
Web of Science (2014): Impact factor 5.426
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.89 SJR 1.744 SNIP 1.296
Web of Science (2013): Impact factor 4.76
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.7 SJR 1.595 SNIP 1.036
Web of Science (2012): Impact factor 3.753
ISI indexed (2012): ISI indexed no
Web of Science (2011): Impact factor
ISI indexed (2011): ISI indexed no
Original language: English
DOIs:
10.1039/C8CY00335A

Research output: Research - peer-review › Journal article – Annual report year: 2018

**Magnetic nickel ferrite nanoparticles as highly durable catalysts for catalytic transfer hydrogenation of bio-based aldehydes**

Magnetic nickel ferrite (NiFe₂O₄) nanoparticles were exploited as stable and easily separable heterogeneous catalysts for catalytic transfer hydrogenation (CTH) of furfural to furfuryl alcohol with 2-propanol as both the hydrogen source and the
solvent providing 94% product yield at 180 degrees C after 6 h of reaction. The magnetic properties of the catalysts provided facile recovery using an external magnet after reaction allowing it to be reused in five reaction cycles without loss of catalytic performance. Importantly, the NiFe₂O₄ nanoparticles were also applicable to CTH of other alkenyl/allyl/aromatic aldehydes affording over 94% selectivity towards the targeted alcohol products, thus being attractive as highly universal catalysts for CTH of aldehydes.

**General information**

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Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, Guizhou University
Contributors: He, J., Yang, S., Riisager, A.
Pages: 790-797
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Peer-reviewed: Yes

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Ratings:
- BFI (2019): BFI-level 2
- Web of Science (2019): Indexed yes
- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
- Web of Science (2017): Impact factor 5.365
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 5.64 SJR 1.811 SNIP 1.287
- Web of Science (2016): Impact factor 5.773
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): CiteScore 5.46 SJR 1.804 SNIP 1.314
- Web of Science (2015): Impact factor 5.287
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): CiteScore 5.44 SJR 1.885 SNIP 1.47
- Web of Science (2014): Impact factor 5.426
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): CiteScore 4.89 SJR 1.744 SNIP 1.296
- Web of Science (2013): Impact factor 4.76
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- Scopus rating (2012): CiteScore 3.7 SJR 1.595 SNIP 1.036
- Web of Science (2012): Impact factor 3.753
- ISI indexed (2012): ISI indexed no
- Web of Science (2011): Impact factor
- ISI indexed (2011): ISI indexed no

Original language: English
DOIs:
10.1039/c7cy02197f
Source: FindIt
Source-ID: 2394878119

Research output: Research - peer-review › Journal article – Annual report year: 2018
Noble metal-free upgrading of multi-unsaturated biomass derivatives at room temperature: Silyl species enable reactivity

Biomass derivatives are a class of oxygen-rich organic compounds, which can be selectively upgraded to various value-added molecules by partial or complete hydrogenation over metal catalysts. Here, we show that Cs₂CO₃, a low-cost commercial chemical, enables the selective reduction of dicarbonyl compounds including bio-derived carboxides to monohydric esters/amides, hydroxylamines or diols with high yields (82-99%) at room temperature using eco-friendly and equivalent hydrosilane as hydride donor. The in-situ formation of silyl ether enables the developed catalytic system to tolerate other unsaturated groups and permits a wide substrate scope with high selectivities. Spectroscopic and computational studies elucidate reaction pathways with an emphasis on the role of endogenous siloxane.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry, Guizhou University, Chinese Academy of Sciences, Tohoku University, Center of Innovative and Applied Bioprocessing
Contributors: Li, H., Zhao, W., Dai, W., Long, J., Watanabe, M., Meier, S., Saravanamurugan, S., Yang, S., Riisager, A.
Number of pages: 8
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Publication information
Journal: Green Chemistry
Volume: 20
Issue number: 23
ISSN (Print): 1463-9262
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Web of Science (2014): Impact factor 8.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
Web of Science (2013): Impact factor 6.852
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.64 SJR 2.444 SNIP 1.701
Web of Science (2012): Impact factor 6.828
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 6.46 SJR 2.32 SNIP 1.641
Web of Science (2011): Impact factor 6.32
Response Factors Enable Rapid Quantitative 2D NMR Analysis in Catalytic Biomass Conversion to Renewable Chemicals

Carbohydrate conversion offers access to a variety of chemicals with diverse functionalities. An accurate analysis of the multiple products in post-reaction material is indispensable for enabling good atom economy in biorefining. A certain need for reconsidering current analytical approaches to chemocatalytic biomass conversion is witnessed by the often poor carbon balances that are reported for carbohydrate conversion processes. Carbohydrate conversion usually includes isomerization and/or dehydration, therefore analytical approaches that are suitable for the distinction and concurrent quantification of isomers are desirable for developing sustainable processes towards known and new chemicals. Quantitative 1D NMR spectroscopy can be used to determine absolute concentrations in the absence of purified reference compounds and can thereafter be used to obtain response factors in other analytical methods resolving the compounds of interest. Here, we show that this approach is applicable for obtaining response factors relative to an internal standard for rapid, highly resolved 2D NMR spectra at natural isotopic abundance. Following calibration, this approach provides a limit of quantification in the order of 0.8 mM within an experiment time of a few minutes. The approach is particularly beneficial for the quantification of compounds at low concentrations, for instance in initial rate experiments, and for the quantification of low populated reaction intermediates.

General information
State: Accepted/In press
Organisations: Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Elliot, S. G., Tosi, I., Riisager, A., Taarning, E., Meier, S.
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ISSN (Print): 1022-5528
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Selective Hydrodeoxygenation of Alkyl Lactates to Alkyl Propionates with Fe-based Bimetallic Supported Catalysts

Hydrodeoxygenation (HDO) of methyl lactate (ML) to methyl propionate (MP) was performed with various base-metal supported catalysts. A high yield of 77% MP was obtained with bimetallic Fe-Ni/ZrO₂ in methanol at 220°C and 50 bar H₂. A synergistic effect of Ni increased the yield of MP significantly when using Fe-Ni/ZrO₂ instead of Fe/ZrO₂ alone. Moreover, the ZrO₂ support contributed to improve the yield as a phase transition of ZrO₂ from tetragonal to monoclinic occurred after metal doping giving rise to fine dispersion of the Fe and Ni on the ZrO₂, resulting in a higher catalytic activity of the material. Interestingly, it was observed that Fe-Ni/ZrO₂ also effectively catalyzed methanol reforming to produce H₂ in situ, followed by HDO of ML, yielding 60% MP at 220°C with 50 bar N₂ instead of H₂. Fe-Ni/ZrO₂ also catalyzed HDO of other short-chain alkyl lactates to the corresponding alkyl propionates in high yields around 70%. No loss of activity of Fe-Ni/ZrO₂ occurred in five consecutive reaction runs demonstrating the high durability of the catalyst system.

General information
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Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Organic Chemistry, Guizhou University
Contributors: Khokarale, S. G., He, J., Schill, L., Yang, S., Riisager, A., Saravanamurugan, S.
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Impact factor 7.411
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Impact factor 7.226
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 7.33 SJR 2.53 SNIP 1.424
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 7.97 SJR 2.864 SNIP 1.663
Web of Science (2014): Impact factor 7.657
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 6.79 SJR 2.561 SNIP 1.46
Web of Science (2013): Impact factor 7.117
ISI indexed (2013): ISI indexed yes
Selective Oxidative Carbonylation of Aniline to Diphenylurea with Ionic Liquids

A catalytic system for the selective oxidative carbonylation of aniline to diphenylurea based on Pd complexes in combination with imidazolium ionic liquids is presented. Both oxidants, Pd complexes and ionic liquids affect the activity of the reaction while the choice of oxidant determines the selectivity of the reaction. Together they allow the reaction to proceed under comparatively mild conditions without loss of activity. In-situ NMR examination of the reaction led to the observation of a previously suggested intermediate supporting the proposed mechanism.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Universidad Rovira i Virgili
Contributors: Zahrtmann, N., Claver, C., Godard, C., Riisager, A., Garcia Suárez, E. J.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.47 SJR 1.695 SNIP 0.925
PROCESS FOR HYDROGENOLYSIS OF ALPHA-HYDROXY ESTERS OR ACIDS USING A HETEROGENEOUS CATALYST

The present invention relates to a method for hydrogenolysis of alpha-hydroxy esters or acids, comprising reacting the alpha-hydroxy ester or acid in the presence of a heterogeneous catalyst. The present invention also relates to a method for producing propionic acid ester, and the use of any of the methods for the production of propionic acid esters, such as alkyl propionate.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Saravanamurugan, S., Khokarale, S. G., Riisager, A.
Publication date: 5 Jan 2017

Publication information
IPC: C07C 67/327 A1
Patent number: WO2017001285
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Priority date: 25/06/2015
Priority number: EP20150173952
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A Pd-Catalyzed in situ domino process for mild and quantitative production of 2,5-dimethylfuran directly from carbohydrates

An in situ domino process has been developed to be highly efficient for direct and mild conversion of various hexose sugars to the biofuel 2,5-dimethylfuran in almost quantitative yields, without separation of unstable intermediates at 120 °C in n-butanol, by using polymethylhydrosiloxane and hydrophobic Pd/C as a H-donor and a bifunctional catalyst, respectively. Among the cascade reactions, the hydrosilylation process was confirmed by deuterium-labeling and kinetic studies to be favorable for sugar dehydration and exclusively acts on deoxygenation of in situ formed intermediates including furanic alcohols and aldehydes to DMF via a hydride transfer process that was facilitated by an alcoholic solvent. The catalytic system is more selective than the H₂-participated counterpart, and could be scaled up with only 0.04 mol% catalyst loading, giving DMF in a comparable yield of 85%. Moreover, Pd(0) was demonstrated to be the active species for deoxygenation, and the heterogeneous catalyst exhibited good recyclability with little elemental leaching.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Guizhou University, Center of Innovative and Applied Bioprocessing, Nanjing Agricultural University
Contributors: Li, H., Zhao, W., Riisager, A., Saravanamurugan, S., Wang, Z., Fang, Z., Yang, S.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Web of Science (2014): Impact factor 8.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
Web of Science (2013): Impact factor 6.852
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Carbon-Increasing Catalytic Strategies for Upgrading Biomass into Energy-Intensive Fuels and Chemicals

Lignocellulosic biomass is the most abundant organic carbon source and has received a great deal of interest as renewable and sustainable feedstock for the production of potential biofuels and value-added chemicals with a wide range of designed catalytic systems. However, those natural polymeric materials are composed of short-chain monomers (typically C₆ and C₅ sugars) and complex lignin molecules containing plenty of oxygen, resulting in products during the downstream processing having low-grade fuel properties or limited applications in organic syntheses. Accordingly, approaches to increase the carbon-chain length or carbon atom number have been developed as crucial catalytic routes for upgrading biomass into energy-intensive fuels and chemicals. The primary focus of this review is to systematically describe the recent examples on the selective synthesis of long-chain oxygenates via different C-C coupling catalytic processes, such as Aldol condensation, hydroalkylation/alkylation, oligomerization, ketonization, Diels-Alder, Guerbet and acylation reactions. Other integrated reaction steps including e.g., hydrolysis, dehydration, oxidation, partial hydrogenation and hydrodeoxygenation (HDO) to derive corresponding key intermediates or final products are also reviewed. The effects of catalyst structure/type and reaction parameters on the catalytic performance along with relevant reaction mechanisms are in detail discussed. Apart from this, the formation of other useful compounds containing C-X bonds (X = O, N and S) derived from biomass-based substrates for producing fuel additives and valuable chemicals is also briefly reviewed.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Guizhou University, Centre of Innovative and Applied Bioprocessing, CSIR Indian Institute of Toxicology Research, University of Córdoba
Contributors: Li, H., Riisager, A., Saravanamurugan, S., Pandey, A., Sangwan, R. S., Yang, S., Luque, R.
Pages: 148-187
Catalytic Transfer Hydrogenation of Furfural to Furfuryl Alcohol with Recyclable Al-Zr@Fe Mixed Oxides

A series of magnetic, acid/base bifunctional Al–Zr@Fe$_3$O$_4$ catalysts were successfully prepared by a facile coprecipitation method and utilized in the catalytic transfer hydrogenation (CTH) of furfural to furfuryl alcohol with 2-propanol as hydrogen source. The physicochemical properties and morphologies of the as-prepared catalysts were characterized by various techniques, including XRD analysis, N2 physisorption, vibrating sample magnetometry, thermal gravimetry analysis, X-ray fluorescence spectroscopy, NH$_3$/CO$_2$ temperature-programmed desorption, SEM, and TEM. The Al$_7$Zr$_3$@Fe$_3$O$_4$(1/1) catalyst with a Al$_{27}$Zr$_{18}$Fe$_{30}$O$_{4}$ molar ratio of 21:9:3 was found to exhibit a high furfuryl alcohol yield of 90.5 % in the CTH from furfural at 180 °C after 4 h with a comparatively low activation energy of 45.3 kJ mol$^{-1}$, as calculated from the Arrhenius equation. Moreover, leaching and recyclability tests confirmed Al$_7$Zr$_3$@Fe$_3$O$_4$(1/1) to function as a heterogeneous catalyst that could be reused for at least five consecutive reaction runs without significant loss of catalytic activity after simple recovery by an external magnet. Notably, the catalyst proved also efficient for hydrogenation of other biomass-derived furanic aldehydes.
Chemoselective Synthesis of Dithioacetals from Bio-aldehydes with Zeolites under Ambient and Solvent-free Conditions

Dithioacetals are an important class of versatile compounds extensively applied in pharmaceuticals, separations, electrochemistry, and organic synthesis, but few heterogeneous catalytic systems are reported to be generally applicable for their synthesis from a wide range of substrates. A series of commercial and modified zeolites are excellent catalysts for thioacetalization of different thiols with carbonyl compounds, including biomass-derived aldehydes, at room temperature under solvent-free conditions. A near quantitative yield of dithioacetal was obtained over H-beta(19) at room temperature with a low catalyst to substrate ratio of 1:19, and a method to follow the reaction progress by ex situ UV/Vis absorption analysis was demonstrated. Recycling experiments with H-beta(19) in five consecutive runs resulted in slight loss of activity, but the original activity could be fully restored after calcination at 550 degrees C. The results and physicochemical properties of the zeolites revealed that relatively large pores and moderate acidity with an appropriate distribution of Bronsted/Lewis acid sites contributed to the pronounced performance in the dithioacetal formation.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Guizhou University, Center of Innovative and Applied Bioprocessing
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Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 4.47 SJR 1.695 SNIP 0.925
Web of Science (2017): Impact factor 4.674
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.33 SJR 1.679 SNIP 0.952
Web of Science (2016): Impact factor 4.803
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.57 SJR 1.731 SNIP 0.996
Web of Science (2015): Impact factor 4.724
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.52 SJR 1.89 SNIP 1.103
Web of Science (2014): Impact factor 4.556
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.82 SJR 2.182 SNIP 1.057
Web of Science (2013): Impact factor 5.044
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 4.58 SJR 2.394 SNIP 1.141
Web of Science (2012): Impact factor 5.181
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 4.3 SJR 2.229 SNIP 1.069
Convenient and Sustainable Hydrogen Storage using Liquid Organic Hydrogen Carrier (LOHC) Technologies

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Søgaard, A., Riisager, A., Bösmann, A., Wasserscheid, P.
Number of pages: 1
Publication date: 2017

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Research output: Research - peer-review » Conference abstract in proceedings – Annual report year: 2017

Facile and Benign Conversion of Sucrose to Fructose Using Zeolites With Balanced Brønsted and Lewis Acidity
Sucrose is by far the industrially most abundant simple carbohydrate with a production volume of more than 160 million metric tons from sugar cane and sugar beet per year. Many promising pathways towards bio-based organic compounds use, however, fructose as the pathway substrate. Hence, a chemocatalytic approach to convert sucrose into fructose would provide a means to channel sucrose into pathways for sugar valorization. Here, we show that a variety of heterogeneous zeolite catalysts with balanced Brønsted and Lewis acidity enable a simple route for the conversion of sucrose to more than 80% fructosides or fructose at 100 °C. The catalysts can encompass aluminum or tin Lewis acidic sites in various zeolite frameworks. The reaction proceeds in volatile alcohol solvents and broadly enables the channelling of sucrose into processes that use fructose as the pathway substrate.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS, Technical University of Denmark
Contributors: Shunmugavel, S., Tosi, I., Rasmussen, K. H., E. Jensen, R., Taarning, E., Meier, S., Riisager, A.
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Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
Giant tunability of the two-dimensional electron gas at the interface of γ-Al₂O₃/SrTiO₃

Two-dimensional electron gases (2DEGs) formed at the interface between two oxide insulators provide a rich platform for the next generation of electronic devices. However, their high carrier density makes it rather challenging to control the interface properties under a low electric field through a dielectric solid insulator, i.e. in the configuration of conventional field-effect transistors. To surpass this long-standing limit, we used ionic liquids as the dielectric layer for electrostatic gating of oxide interfaces in an electric double layer transistor (EDLT) configuration. Herein, we reported giant tunability of the physical properties of 2DEGs at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃ (GAO/STO). By modulating the carrier density thus the band filling with ionic-liquid gating, the system experiences a Lifshitz transition at a critical carrier density of 3.0×10¹⁴ cm⁻², where a remarkably strong enhancement of Rashba spin-orbit interaction and an emergence of Kondo effect at low temperatures are observed. Moreover, as the carrier concentration depletes with decreasing gating voltage, the electron mobility is enhanced by more than 6 times in magnitude, leading to the observation of clear quantum oscillations. The great tunability of GAO/STO interface by EDLT gating not only shows promise for design of oxide devices with on-demand properties, but also sheds new light on the electronic structure of 2DEG at the non-isostructural spinel/perovskite interface.
Glucose Isomerization by Enzymes and Chemo-catalysts: Status and Current Advances

The well-known interconversion of aldoses to their corresponding ketoses was discovered more than a century ago, but has recently attracted renewed attention due to alternative application areas. Since the pioneering discovery, much work has been directed toward improving the process of isomerization of aldoses in terms of yields, catalysts, solvents, catalytic systems, etc., by both enzymatic and chemo-catalytic approaches. Among aldose ketose interconversion reactions, fructose production by glucose isomerization to make high-fructose corn syrup (HFCS) is an industrially important and large biocatalytic process today, and a large number of studies have been reported on the process development. In parallel, also alternative chemo-catalytic systems have emerged, as enzymatic conversion has drawbacks, though they are typically more selective and produce fructose under mild reaction conditions. Isomerization of glucose is also a central reaction for making renewable platform chemicals, such as lactic acid, 5-hydroxymethylfurfural (HMF), and levulinic acid. In these other applications, thermally stable catalysts are required, thus making use of enzymatic catalysis inadequate, since enzymes generally possess a limited temperature operating window, typically less than 80 °C. From this viewpoint, the chemo-catalysts especially solid heterogeneous catalysts-are playing a key role for the development of not only making HFCS, but also making chemicals and fuels from glucose via the isomerized product/intermediate fructose. This review focuses on how both enzyme and chemo-catalysts are being useful for the isomerization of glucose to fructose. Specifically, development of Lewis acid containing zeolites for glucose isomerization is reviewed in detail, including mechanism, isotopic labeling, and computational studies.
Highly Selective Aerobic Oxidation of 5-Hydroxymethyl Furfural into 2,5-Diformylfuran over Mn-Co Binary Oxides

A series of Mn–Co binary oxides were prepared by a simple thermal decomposition procedure and evaluated for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) into 2,5-diformylfuran (DFF). Investigation of the effects of metal amounts and calcination temperatures of the prepared catalysts revealed that the Mn–Co binary oxide with a Mn/Co molar ratio of 1/1 showed the best catalytic performance yielding 42.6% HMF conversion along with 98% selectivity to DFF after 2 h of reaction. The as-prepared catalysts were characterized by nitrogen physisorption, X-ray powder diffraction (XRD), hydrogen temperature-programmed reduction (H2-TPR) and X-ray photoelectron spectroscopy (XPS). These results indicated that the Mn–Co binary oxides could increase the Mn⁴⁺/Mn³⁺ atomic ratio and the exposed lattice oxygen content on the surface, thus accelerating the HMF oxidation into DFF. Furthermore, the Mn–Co binary oxides proved to be reusable in five consecutive reaction runs without significant loss of activity.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, East China University of Science and Technology
Contributors: Gui, Z., Shunmugavel, S., Cao, W., Schill, L., Chen, L., Qi, Z., Riisager, A.
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Web of Science (2017): Impact factor 1.505
Web of Science (2016): Indexed yes
Web of Science (2015): Impact factor
Original language: English
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Source: FindIt
Source-ID: 2373207049
Research output: Research - peer-review › Journal article – Annual report year: 2017
Highly Selective Continuous Gas-Phase Methoxycarbonylation of Ethylene with Supported Ionic Liquid Phase (SILP) Catalysts

Supported ionic liquid phase (SILP) technology was applied for the first time to the Pd-catalyzed continuous, gas-phase methoxycarbonylation of ethylene to selectively produce methyl propanoate (MP) in high yields. The influence of catalyst and reaction parameters such as, for example, ionic liquid loading, metal concentration, and ligand loadings was studied, and in particular the SILP catalyst activity and stability was found to be strongly dependent on the ligand to metal ratio.

General information

State: Published
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.47 SJR 1.695 SNIP 0.925
Web of Science (2017): Impact factor 4.674
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.33 SJR 1.679 SNIP 0.952
Web of Science (2016): Impact factor 4.803
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.57 SJR 1.731 SNIP 0.996
Web of Science (2015): Impact factor 4.724
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.52 SJR 1.89 SNIP 1.103
Web of Science (2014): Impact factor 4.556
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.82 SJR 2.182 SNIP 1.057
Web of Science (2013): Impact factor 5.044
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 4.58 SJR 2.394 SNIP 1.141
Web of Science (2012): Impact factor 5.181
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): CiteScore 4.3 SJR 2.229 SNIP 1.069
Web of Science (2011): Impact factor 5.207
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 1.689 SNIP 0.925
Web of Science (2010): Impact factor 3.345
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Hydrodeoxygenation of Bio-polymer Precursors with Base Metal Catalysts

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Contributors: Khokarale, S. G., Shunmugavel, S., Riisager, A.
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Hydroformylation with Integrated Catalytic-Membrane Separation Reaction System

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Hydroformylation with Integrated SILP Catalyst-Membrane Separation Reaction System

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Off-Pathway Intermediates in the Conversion of Sugars to Plastic

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS
Contributors: Tosi, I., Riisager, A., Taarning, E., Meier, S.
Number of pages: 1
Publication date: 2017
Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite: a combined DFT/experimental study

The reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite was studied theoretically with periodic density functional theory calculations including dispersion forces and experimentally in a fixed bed flow reactor at pressures between 10 and 100 bar, dimethyl ether concentrations in CO between 0.2 and 2.0%, and at a temperature of 438 K. The theoretical study showed that the reaction of CO with surface methyl groups, the rate-limiting step, is faster in the eight-membered side pockets than in the twelve-membered main channel of the zeolite; the subsequent reaction of dimethyl ether with surface acetyl to form methyl acetate was demonstrated to occur with low energy barriers in both the side pockets and in the main channel. The present analysis has thus identified a path, where the entire reaction occurs favourably on a single site within the side pocket, in good agreement with previous experimental studies. The experimental study of the reaction kinetics was consistent with the theoretically derived mechanism and in addition revealed that the methyl acetate product inhibits the reaction - possibly by sterically hindering the attack of CO on the methyl groups in the side pockets.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS, SLAC National Accelerator Laboratory
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
Web of Science (2017): Impact factor 5.365
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.64 SJR 1.811 SNIP 1.287
Web of Science (2016): Impact factor 5.773
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.46 SJR 1.804 SNIP 1.314
Web of Science (2015): Impact factor 5.287
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.44 SJR 1.885 SNIP 1.47
Web of Science (2014): Impact factor 5.426
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Rhodium Catalyzed Decarbonylation

Rhodium catalyzed decarbonylation has developed significantly over the last 50 years and resulted in a wide range of reported catalyst systems and reaction protocols. Besides experimental data, literature also includes mechanistic studies incorporating Hammett methods, analysis of kinetic isotope effects as well as computational studies of model systems, which give an indication of the scope of the process. In this chapter, fundamental applications of Rh-catalyzed decarbonylation reactions are surveyed and discussed, including cross-coupling reactions, tandem reactions, and alternative methodologies for process intensification.

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Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, Technical University of Denmark
Contributors: Garcia Suárez, E. J., Kahr, K., Riisager, A.
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ROMEO: a new reactor concept for hydroformylation process intensification

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
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Ruthenium Dioxide Catalysts for the Selective Oxidation of Benzylamine to Benzonitrile: Investigating the Effect of Ruthenium Loading on Physical and Catalytic Properties

The oxidative dehydrogenation of benzylamine to benzonitrile was studied in batch and continuous flow processes using ruthenium dioxide catalysts with varying ruthenium loadings. Increased conversions were observed in the continuous flow process compared with the batch process (up to 100% in the flow process compared with up to 92% in the batch process), with increased selectivity to benzonitrile (82 and 65%, respectively) and benzonitrile yields (84 and 58%, respectively). The major by-product was N-benzylidenebenzylamine. The ruthenium loading in the catalyst was successfully optimised and the most active catalyst had a ruthenium loading of 2.5-3.5 wt%.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Nordvang, E. C., Schill, L., Riisager, A., Fehrmann, R.
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BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.57 SJR 0.965 SNIP 0.753
Web of Science (2017): Impact factor 2.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.877
Web of Science (2016): Impact factor 2.486
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.41 SJR 0.926 SNIP 0.777
Web of Science (2015): Impact factor 2.355
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.29 SJR 0.987 SNIP 0.845
Web of Science (2014): Impact factor 2.365
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.67 SJR 1.119 SNIP 0.827
Web of Science (2013): Impact factor 2.22
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.49 SJR 1.196 SNIP 0.848
Web of Science (2012): Impact factor 2.608
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Absorption and oxidation of nitrogen oxide in ionic liquids

A new strategy for capturing nitrogen oxide, NO, from the gas phase is presented. Dilute NO gas is removed from the gas phase by ionic liquids under ambient conditions. The nitrate anion of the ionic liquid catalyzes the oxidation of NO to nitric acid by atmospheric oxygen in the presence of water. The nitric acid is absorbed in the ionic liquid up to approximately one mole HNO₃ per mole of the ionic liquid due to the formation of hydrogen bonds. The nitric acid can be desorbed by heating, thereby regenerating the ionic liquid with excellent reproducibility. Here, time-resolved in-situ spectroscopic investigations of the reaction and products are presented. The procedure reveals a new vision for removing the pollutant NO by absorption into a non-volatile liquid and converting it into a useful bulk chemical, that is, HNO₃.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Thomassen, P. L., Riisager, A., Mossin, S., Fehrmann, R.
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Journal: Chemistry: A European Journal
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ISSN (Print): 0947-6539
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  BFI (2019): BFI-level 2
  Web of Science (2019): Indexed yes
  BFI (2018): BFI-level 2
  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 2
  Scopus rating (2017): CiteScore 4.9 SJR 2.265 SNIP 1.02
  Web of Science (2017): Impact factor 5.16
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.068
  Web of Science (2016): Impact factor 5.317
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): CiteScore 4.99 SJR 2.461 SNIP 1.195
  Web of Science (2015): Impact factor 5.771
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): CiteScore 5.51 SJR 2.526 SNIP 1.222
  Web of Science (2014): Impact factor 5.731
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): CiteScore 5.68 SJR 2.643 SNIP 1.239
  Web of Science (2013): Impact factor 5.696
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): CiteScore 5.55 SJR 2.935 SNIP 1.291
  Web of Science (2012): Impact factor 5.831
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): CiteScore 5.46 SJR 2.902 SNIP 1.319
  Web of Science (2011): Impact factor 5.925
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 2.791 SNIP 1.295
  Web of Science (2010): Impact factor 5.476
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 2
  Scopus rating (2009): SJR 2.753 SNIP 1.425
  Web of Science (2009): Indexed yes
  BFI (2008): BFI-level 2
  Scopus rating (2008): SJR 3.135 SNIP 1.473
  Web of Science (2008): Indexed yes
  Scopus rating (2007): SJR 3.449 SNIP 1.585
  Scopus rating (2006): SJR 3.108 SNIP 1.553
  Web of Science (2006): Indexed yes
  Scopus rating (2005): SJR 2.78 SNIP 1.451
  Web of Science (2005): Indexed yes
Acid-Base Bifunctional Zirconium N-Alkyltriphosphate Nanohybrid for Hydrogen Transfer of Biomass-Derived Carboxides

Catalytic transfer hydrogenation (CTH) reactions are efficient transformation routes to upgrade biobased chemicals. Herein, we report a facile and template-free route to synthesize a series of heterogeneous nitrogen-containing alkyltriphosphonate-metal hybrids with enhancive Lewis acid and base sites, and their catalytic activity in converting biomass-derived carbonyl compounds to corresponding alcohols in 2-propanol. Particularly, a quantitative yield of furfuryl alcohol (FFA) was obtained from furfural (FUR) over organotriphosphate-zirconium hybrid (ZrPN) under mild conditions. The presence of Lewis basic sites adjacent to acid sites with an appropriate base/acid site ratio (1:0.7) in ZrPN significantly improved the yield of FFA. Mechanistic studies for the transformation of FUR to FFA with ZrPN in 2-propanol-d(8) evidently indicate CTH reaction proceeding via a direct intermolecular hydrogen transfer route. It was also found that ZrPN could catalyze isomerization of C-3-C-6 aldoses to ketoses involving intramolecular hydrogen transfer in water.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Guizhou University
Contributors: Li, H., He, J., Riisager, A., Shunmugavel, S., Song, B., Yang, S.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 11.49 SJR 4.921 SNIP 2.113
Web of Science (2017): Impact factor 11.384
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.367 SNIP 2.081
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Atomically thin Pt shells on Au nanoparticle cores: facile synthesis and efficient synergetic catalysis

We present a facile synthesis protocol for atomically thin platinum (Pt) shells on top of gold (Au) nanoparticles (NPs) (Au@PtNPs) in one pot under mild conditions. The Au@PtNPs exhibited remarkable stability (> 2 years) at room temperature. The synthesis, bimetallic nanostructures and catalytic properties were thoroughly characterized by ultraviolet-visible light spectrophotometry, transmission electron microscopy, nanoparticle tracking analysis and electrochemistry. The 8 ± 2 nm Au@PtNPs contained 24 ± 1 mol% Pt and 76 ± 1 mol% Au corresponding to an atomically thin Pt shell. Electrochemical data clearly show that the active surface is dominated by Pt with a specific surface area above 45 m² per gram of Pt. Interactions with the Au core increase the activity of the Pt shell by up to 55% and improve catalytic selectivity compared to pure Pt. The Au@Pt NPs show exciting catalytic activity in electrooxidation of sustainable fuels (i.e. formic acid, methanol and ethanol), and selective hydrogenation of benzene derivatives. Especially high activity was achieved for formic acid oxidation, 549 mA (mgPt)−1 (at 0.6 V vs. SCE), which is 3.5 fold higher than a commercial < 5 nm PtNP catalyst. Excellent activity for the direct production of γ-valerolactone, an alternative biofuel/fuel additive, from levulinic acid and methyl levulinate was finally demonstrated.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Engelbrekt, C., Seselj, N., Poreddy, R., Riisager, A., Ulstrup, J., Zhang, J.
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ISSN (Print): 2050-7488
Ratings:
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Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Brønsted Acid Ionic Liquids (BAILs) as Efficient and Recyclable Catalysts in the Conversion of Glycerol to Solketal at Room Temperature

Brønsted acid ionic liquids (BAILs) have been prepared and applied for the first time - to the best of our knowledge - as efficient catalysts in the acetylation of glycerol with acetone to form solketal ((2,2-dimethyl-1,3-dioxolan-4-yl)methanol) at very mild reaction conditions (room temperature) and short reaction times. The BAILs showed a superior catalytic performance in terms of both conversion and selectivity compared to the common mineral acid methanesulfonic acid as well as to other reported homogeneous and heterogeneous catalysts. Catalyst reusability was demonstrated with one of the BAILs (BAIL-1), which was recovered and reused by a simple procedure in four consecutive reaction runs without any loss of catalytic activity and selectivity. Thus, the BAILs combine the advantages of both homogeneous and heterogeneous catalysis with respect to excellent conversion and selectivity as well as easy recyclability.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Technical University of Denmark, Catalytic Spectroscopy Laboratory, East China University of Science and Technology
Contributors: Gui, Z., Zahrtmann, N., Shunmugavel, S., Reyero, I., Qi, Z., Bañares, M. A., Riisager, A., Garcia-Suarez, E. J.
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Chemoselective hydrogenation of arenes by PVP supported Rh nanoparticles

Polyvinylpyrrolidone-stabilized Rh nanoparticles (RhNPs/PVP) of ca. 2.2 nm in size were prepared by the hydrogenation of the organometallic complex [Rh(η3-C3H5)3] in the presence of PVP and evaluated as a catalyst in the hydrogenation of a series of arene substrates as well as levulinic acid and methyl levulinate. The catalyst showed excellent activity and selectivity towards aromatic ring hydrogenation compared to other reported transition metal-based catalysts under mild reaction conditions (room temperature and 1 bar H2). Furthermore, it was shown to be a highly promising catalyst for the hydrogenation of levulinic acid and methyl levulinate in water leading to quantitative formation of the fuel additive γ-valerolactone under moderate reaction conditions compared to previously reported catalytic systems.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, CNRS, Universite de Toulouse
Contributors: Ibrahim, M., Poreddy, R., Philippot, K., Riisager, A., Garcia-Suarez, E. J.
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.93 SJR 1.306 SNIP 0.904
Web of Science (2017): Impact factor 4.099
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.85 SJR 1.229 SNIP 0.918
Web of Science (2016): Impact factor 4.029
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.1 SJR 1.302 SNIP 1.006
Web of Science (2015): Impact factor 4.177
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.06 SJR 1.389 SNIP 1.064
Web of Science (2014): Impact factor 4.197
Web of Science (2014): Indexed yes
Combined Function of Brønsted and Lewis Acidity in the Zeolite-Catalyzed Isomerization of Glucose to Fructose in Alcohols

Glucose conversion via fructose to useful chemicals and fuels has attracted considerable attention. Isomerization of glucose to fructose can proceed along several different reaction pathways involving different sugar intermediates and isomeric forms. Presently, the roles of the substrate isomeric forms and of the catalyst properties remain incompletely understood. By using NMR spectroscopy, we elucidate the interplay of the catalyst active sites in converting monosaccharide forms to products, byproducts, and intermediates in alcohols.
### General information
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Organisations: Organic Chemistry, Department of Chemistry, Haldor Topsoe AS  
Contributors: Shunmugavel, S., Riisager, A., Taarning, E., Meier, S.  
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BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 4.47 SJR 1.695 SNIP 0.925  
Web of Science (2017): Impact factor 4.674  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 4.33 SJR 1.679 SNIP 0.952  
Web of Science (2016): Impact factor 4.803  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): CiteScore 4.57 SJR 1.731 SNIP 0.996  
Web of Science (2015): Impact factor 4.724  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): CiteScore 4.52 SJR 1.89 SNIP 1.103  
Web of Science (2014): Impact factor 4.556  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): CiteScore 4.82 SJR 2.182 SNIP 1.057  
Web of Science (2013): Impact factor 5.044  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
Scopus rating (2012): CiteScore 4.58 SJR 2.394 SNIP 1.141  
Web of Science (2012): Impact factor 5.181  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
Scopus rating (2011): CiteScore 4.3 SJR 2.229 SNIP 1.069  
Web of Science (2011): Impact factor 5.207  
ISI indexed (2011): ISI indexed no  
Scopus rating (2010): SJR 1.689 SNIP 0.925  
Web of Science (2010): Impact factor 3.345  
Web of Science (2010): Indexed yes  

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Direct transformation of carbohydrates to the biofuel 5-ethoxymethylfurfural by solid acid catalysts

The direct conversion of glucose to 5-ethoxymethylfurfural (EMF) is a promising biomass transformation due to the products potential application as a biofuel. Here, the conversion of glucose to EMF was examined over several solid acid catalysts in ethanol between 96 and 125 oC. Among the catalysts employed, dealuminated beta zeolites [DeAl-H-beta-12.5 (700)] gave a moderate yield of EMF (37%) in a single step catalytic process. A combined catalytic system consisting of H-form zeolite and Amberlyst-15 was found to be more efficient for the transformation of glucose to EMF (46%) via an one-pot, two-step reaction protocol. Alternative biomass-based mono-, di- and polysaccharides formed also moderate to good yields of EMF with the catalytic systems, including fructose which yielded 67 % of EMF and 4% of ethyl levulinate (ELevu) along with 10 % 5-hydroxymethylfurfural (HMF) in the combined reaction protocol. A significant amount of ELevu (1-16 %), a rehydrated product of EMF and promising fuel additive, was observed in this study. Recyclability studies suggested that it was possible to reuse the DeAl-H-beta-12.5 (700) catalyst in consecutive reactions without significant changes in product yields due to its easy recovery and thermal stability during regeneration.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, Guizhou University
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BFI (2019): BFI-level 2
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Web of Science (2014): Impact factor 8.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
Web of Science (2013): Impact factor 6.852
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.64 SJR 2.444 SNIP 1.701
Web of Science (2012): Impact factor 6.828
Efficient Aerobic Oxidation of 5-Hydroxymethylfurfural in Aqueous Media with Au-Pd Supported on Zinc Hydroxycarbonate

Bimetallic catalysts with Au–Pd supported on zinc hydroxycarbonate (ZOC) were synthesized by a simple deposition–precipitation method and analyzed by transmission electron microscopy to have a narrow-size distribution of predominantly 1–2 nm. The prepared Au–Pd/ZOC catalysts exhibited excellent activity towards 5-hydroxymethylfurfural (HMF) oxidation in water in the presence of the base NaHCO3 at benign conditions of 80 °C and 3 bar O2, resulting in quantitative yield of 2,5-furandicarboxylic acid (FDCA). The addition of base not only enhanced the yield of FDCA but also stabilized the support ZOC by preventing ZOC from the reaction with formed carboxylic acid intermediates/products, thus allowing Au–Pd/ZOC to be recycled for at least six times without significant loss of activity. The basicity of ZOC could play an important role in obtaining the improved yield of FDCA as compared to other supports.

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Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, East China University of Science and Technology
Contributors: Gui, Z., Cao, W., Shunmugavel, S., Riisager, A., Chen, L., Qi, Z.
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Lignin biomass conversion into chemicals and fuels

Second-generation biomass or lignocellulosic biomass, which is mainly composed of cellulose, hemicellulose and lignin, is a very important and promising feedstock for the renewable production of fuels and chemicals of the future. Lignin is the second most abundant natural polymer, representing 30% of the weight and 40% of the energy content of lignocellulosic biomass. While designated applications for cellulose already exist in form of the current pulp and paper production as well as its prospective hydrolysis and fermentation into biofuels (mainly bioethanol), sustainable ways to valorize the lignin fraction of wood are yet to be established, due to its poor solubility and complex heterogeneous structure. This constitutes a major drawback in the economic viability of a biorefinery, where complete valorization of lignocellulosic biomass is necessary. For this reason, and due to its potential as a valuable feedstock for the production of organic chemicals, lignin valorization has become an important issue to solve.

For a better understanding and analysis of the catalytic performance of lignin, it is common to use lignin model compounds, which contain the most significant linkages present in lignin and show similar, although simplified, characteristics to the natural biopolymer. Among them, the most abundant structural unit is the β-O-4, representing approximately 60% of the bonds in hardwood and 45-50% of those in softwood.
Oxidative depolymerization is one of the most viable methods for lignin valorization. It involves the cleavage of ether bonds, such as β-O-4 and other linkages present in lignin and its model compounds, giving aldehydes or carboxylic acids as products, depending on the reaction conditions used. In Chapter 2 of this thesis, the preparation, characterization and catalytic performance of heterogeneous catalysts for the aerobic oxidation of β-O-4 lignin model compounds (veratryl alcohol and guaiacyl glycerol-β-guaiacyl ether) is discussed.

The use of an environmentally friendly process, the organosolv process, for treating lignocellulosic biomass in the presence of a solvent and using reaction conditions under which at least part of the lignin is separated from the biomass, is described in Chapter 3. Different catalysts and reaction conditions have been studied in order to optimize the organosolv process for the production of high-quality lignin for further upgrading.

At the end of this thesis, Chapter 4, a catalytic process is described for the valorization of lignin, consisting of a two-step catalytic system. The two-step catalytic system involved catalytic oxidation, followed by hydrogenolysis. A catalytic system was developed for lignin hydrogenolysis and the influence of the temperature and reaction time was studied for the catalytic oxidation of lignin.

The results presented in this thesis contribute to a better understanding of the various factors influencing the production of bulk aromatic chemicals from lignin, including valuable knowledge regarding catalyst activity and stability, optimal conditions for the valorization of lignin and lignin model compounds, and a process for the extraction of lignin from wood. Hence, it is necessary to further develop catalytic processes to enable the transformation of lignin from a low quality, low-price waste product into a high-quality, high-value feedstock for bulk and specialty chemicals by the development of the appropriate catalytic technology.

This transformation is critical because lignin represents the only viable renewable source to produce the aromatic compounds on which society currently depends.

**Mechanism and Stereoselectivity of Zeolite-catalysed Sugar Isomerisation in Alcohols**

Glucose isomerisation to fructose can occur by different pathways and the mechanism of zeolite-catalysed glucose isomerisation in methanol has remained incompletely understood. Herein, the mechanism is studied using an 1H-13C HSQC NMR assay resolving different fructose isotopomers. We find that zeolite-catalysed glucose isomerisation proceeds predominantly via a hydride shift into the pro-R position of fructose, thus resembling the stereoselectivity of the enzymatic isomerisation process.
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127
Web of Science (2017): Impact factor 6.29
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.06 SJR 2.538 SNIP 1.16
Web of Science (2016): Impact factor 6.319
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.7 SJR 2.601 SNIP 1.295
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.83 SJR 2.692 SNIP 1.436
Web of Science (2014): Impact factor 6.834
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.73 SJR 2.752 SNIP 1.372
Web of Science (2013): Impact factor 6.718
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.21 SJR 3.118 SNIP 1.35
Web of Science (2012): Impact factor 6.378
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.96 SJR 2.889 SNIP 1.323
Web of Science (2011): Impact factor 6.169
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.781 SNIP 1.255
Web of Science (2010): Impact factor 5.787
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.669 SNIP 1.31
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.909 SNIP 1.286
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.957 SNIP 1.278
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.487 SNIP 1.264
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.265 SNIP 1.225
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.071 SNIP 1.251
Scopus rating (2003): SJR 1.828 SNIP 1.2
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.04 SNIP 1.29
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.036 SNIP 1.215
Methoxycarbonylation of alkenes with biomass-derived CO

The production of chemicals, fuels and energy from renewable feedstock, such as biomass, has seen increasing interest in the last decade. One of the key issues regarding biorenewables is the reduction of the oxygenation grade in molecules, the removal of oxygen. This thesis focuses on the removal of oxygen, in the form of carbon monoxide, and use in a tandem reaction for the methoxycarbonylation of alkenes. Furthermore, the production of γ-valerolactone (GVL), a promising green fuel has been exploited.

Chapter 1: Introduction provides a walk-through of subjects like biomass and its utility, dehydration of sugars, the importance of the furanoic platform and carbonylation reactions. All these arguments are described in detail, taking into account the current and past research, accurately chosen in order to offer an insight for next chapters.

Chapter 2: Experimental, deals with the analytical techniques and the catalytic setups of the reactions. Chapter 3: Results and Discussion, is divided into two main parts. The first one reports and discuss the data obtained after the methoxycarbonylation reaction of 5 HMF (5-hydroxymethyl furfural), to yield methyl heptanoate (MH), methyl levulinate (ML), and GVL, the three products we investigated. The catalytic system is optimized, following the indication given by the results of the reactions. All the steps of the process are deeply discussed in this section. Consideration on the reaction time, on the choice and the quantity of the acidic catalyst, the nature and the amount of the palladium precursor and the phosphine ligand, a screening of the reaction temperatures, and an investigation regarding different substrates (with a furanic backbone), alkenes and alcohols have been done. Our catalytic system proved to be valid to give good yields in a one-pot reaction from HMF to valuable products. All the data are gathered after GC-FID, GS-MS and HPLC analysis, run using naphthalene as internal standard. The second part examines the methoxycarbonylation reaction applied to different carbohydrates. Insights on the kinetics of the reaction and the reactivity of various carbohydrates can be inferred from the analysis of the reported data. Through this screening, our catalytic system proved to be active on a broad range sugars, from monosaccharides to polysaccharides, such as inulin and starch. Chapter 4: Conclusions, it summarizes the results, future perspectives and possible developments.
Selective Reversible Absorption of the Industrial Off-Gas Components CO$_2$ and NO$_x$ by Ionic Liquids

Ionic liquids are promising new materials for climate and pollution control by selective absorption of CO$_2$ and NO$_x$ in industrial off-gases. In addition practical cleaning of industrial off gases seems to be attractive by use of ionic liquids distributed on the surface of porous, high surface area carriers in the form of so-called Supported Ionic Liquid Phase (SILP) materials. The potential of selected ionic liquids for absorption of CO$_2$ and NO$_x$ are demonstrated and the possible interference of other gases influencing the stability and absorption capacity of the ionic liquids are investigated as well.
Selective Reversible Absorption of the Industrial Off-Gas Components CO$_2$ and NO$_x$ by Ionic Liquids

Ionic liquids are promising new materials for climate and pollution control by selective absorption of CO$_2$ and NO$_x$ in industrial off-gases. In addition practical cleaning of industrial off gases seems to be attractive by use of ionic liquids distributed on the surface of porous, high surface area carriers in the form of so-called Supported Ionic Liquid Phase (SILP) materials. The potential of selected ionic liquids for absorption of CO$_2$ and NO$_x$ will be demonstrated and the possible mechanism of absorption will be described on the molecular level. Our vision of application of these ionic liquids in the form of SILP filters to flue gas cleaning in power plants, waste incineration plants, cement and glass factories as well as unborad ships will be adressed.

Synergy Effects of the Mixture of Bismuth Molybdate Catalysts with SnO2/ZrO2/MgO in Selective Propene Oxidation and the Connection between Conductivity and Catalytic Activity

Bismuth molybdate catalysts have been used for partial oxidation and ammoxidation of light hydrocarbons since the 1950s. In particular, there is the synergy effect (the enhancement of the catalytic activity in the catalysts mixed from different components) in different phases of bismuth molybdate catalysts which has been observed and studied since the 1980s; however, despite it being interpreted differently by different research groups, there is still no decisive conclusion on the origin of the synergy effect that has been obtained. The starting idea of this work is to find an answer for the question: does the electrical conductivity influence the catalytic activity (which has been previously proposed by some authors). In this work, highly conductive materials (SnO$_2$, ZrO$_2$) and nonconductive materials (MgO) are added to beta bismuth molybdates (beta-Bi$_2$Mo$_2$O$_9$) using mechanical mixing, impregnation, and sol-gel methods. The mixtures were characterized by XRD, BET, XPS, and EDX techniques to determine the phase composition and surface properties. The conductivities of these samples were recorded at the catalytic reaction temperature (300-450 degrees C). Comparison of the catalytic activities of these mixtures showed that the addition of 10% mol SnO$_2$ to beta bismuth molybdate resulted in the highest activity while the addition of nonconductive MgO could not increase the catalytic activity. This shows that there may be a connection between conductivity and catalytic activity in the mixtures of bismuth molybdate catalysts and other metal oxides.
Ratings:

BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.4 SJR 0.978 SNIP 1.203
Web of Science (2017): Impact factor 3.141
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.95 SNIP 1.155
Web of Science (2016): Impact factor 2.843
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.87 SJR 0.938 SNIP 1.145
Web of Science (2015): Impact factor 2.567
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.85 SJR 1.009 SNIP 1.287
Web of Science (2014): Impact factor 2.587
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.6 SJR 0.975 SNIP 1.232
Web of Science (2013): Impact factor 2.235
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.56 SJR 1.054 SNIP 1.32
Web of Science (2012): Impact factor 2.206
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 2.58 SJR 1.076 SNIP 1.236
Web of Science (2011): Impact factor 2.237
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.049 SNIP 1.161
Web of Science (2010): Impact factor 2.072
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.001 SNIP 1.156
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.14 SNIP 1.255
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.106 SNIP 1.233
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.035 SNIP 1.209
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.992 SNIP 1.231
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.044 SNIP 1.448
Tin-Containing Silicates: Identification of a Glycolytic Pathway via 3-Deoxyglucosone

Inorganic glycolytic systems, capable of transforming glucose through a cascade of catalytic steps, can lead to efficient chemical processes utilising carbohydrates as feedstock. Tin-containing silicates, such as Sn-Beta, are showing potential for the production of lactates from sugars through a cascade of four to five sequential steps. Currently, there is a limited understanding of the competing glycolytic pathways within these systems. Here we identify dehydration of glucose to 3-deoxyglucosone as an important pathway that occurs in addition to retro-aldol reaction of hexoses when using tin-containing silicates. It is possible to influence the relative carbon flux through these pathways by controlling the amount of alkali metal salts present in the reaction mixture. In the absence of added potassium carbonate, at least 15–30% carbon flux via 3-deoxyglucosone is observed. Addition of just a few ppm of potassium carbonate makes retro-aldol pathways dominant and responsible for about 60-70% of the overall carbon flux. The 3-deoxyglucosone pathway results in new types of chemical products accessible directly from glucose. Furthermore, it is argued that 3-deoxyglucosone is a contributing source of some of the methyl lactate formed from hexoses using tin-containing silicates in the presence of alkali metal salts. Further catalyst design and system tuning will permit even better control between these two different glycolytic pathways and will enable highly selective catalytic transformations of glucose to a variety of chemical products using tin-containing silicates.

General information

State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry, Aarhus University, Haldor Topsoe AS
Contributors: Tolborg, S., Meier, S., Sádaba, I., Elliot, S. G., K. Kristensen, S., Shunmugavel, S., Riisager, A., Fristrup, P., Skrydstrup, T., Taarning, E.
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Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
Zeolite and zeotype-catalysed transformations of biofuranic compounds
Catalytic valorisation of biomass with solid functional materials has been recognised as a promising approach to produce value-added biochemicals and biofuels. Furanic compounds such as 5-hydroxymethylfurfural (HMF), 5-ethoxymethylfurfural, 2,5-dimethylfuran, 2,5-diformylfuran and 2,5-furandicarboxylic acid can be obtained from hexoses and pentoses via selective dehydration and subsequent etherification, hydrogenation, oxidation reactions, which show...
great potential for industrial applications to replace petroleum-based chemicals and fuels. Zeolite and zeotype micro- and mesoporous materials with tuneable acidity, good thermal stability and shape-selectivity have recently emerged as promising solid catalysts, exhibiting superior catalytic performance to other heterogeneous catalysts. This review focuses on the synthesis of biomass-derived furanic compounds catalysed by zeolitic materials, firstly introducing zeolite-catalysed hydrolysis of di-, oligo- and polysaccharides and isomerization reactions of monomeric sugars. Subsequently, the catalytic dehydration reactions of hexoses and pentoses to obtain HMF and furfural are reported. Particularly, a variety of reaction pathways towards upgrading of the resulting platform furanic molecules to valuable bioproducts over zeolitic materials are discussed.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Guizhou University, Centre of Innovative and Applied Bioprocessing, University of Córdoba
Contributors: Li, H., Yang, S., Riisager, A., Pandey, A., Sangwan, R. S., Saravanamurugan, S., Luque, R.
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Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Web of Science (2014): Impact factor 8.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
Web of Science (2013): Impact factor 6.852
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.64 SJR 2.444 SNIP 1.701
Web of Science (2012): Impact factor 6.828
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 6.46 SJR 2.32 SNIP 1.641
Web of Science (2011): Impact factor 6.32
Zeolite-catalyzed conversion of sucrose to fructose

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, Technical University of Denmark, Haldor Topsoe AS
Contributors: Shunmugavel, S., Tosi, I., H. Rasmussen, K., E. Jensen, R., Taarning, E., Meier, S., Riisager, A.
Number of pages: 1
Publication date: 2016
Peer-reviewed: Yes
URLs:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract R-10
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Combined oxidation and absorption of nox by an ionic liquid tandem process.
The present invention relates to a new strategy for capturing NOx using a two-step process.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, DTU Admission Course, Office for Research and Relations, Risø National Laboratory for Sustainable Energy
Publication date: 22 Oct 2015

Publication information
Aerobic Oxidation of Veratryl Alcohol to Veratraldehyde with Heterogeneous Ruthenium Catalysts

Lignin is a complex polymeric molecule constituting various linkages between aromatic moieties. Typically, the β-O-4 linkage accounts for more than half of the linkage structures present in lignin. The current study focuses on the oxidative transformation of veratryl alcohol (VA)—a compound that can be formed by cleavage of β-O-4 linkages in lignin—to veratraldehyde (VAld) with air using ruthenium supported on γ-alumina or silica as catalyst with water or methanol as solvent in a batch reactor. Ru/Al₂O₃, prepared with ruthenium(IV)oxide hydrate showed superior catalytic activity, yielding 89 % VAld in water at 160 °C with 5 bar air pressure after 8 h of reaction. Prolonged reaction time led to significant formation of the decarbonylated product veratrol from VAld. When the reaction was completed under 20 bars of argon in methanol instead of water, the methyl ether of VA (i.e. 1,2-dimethoxy-4-(methoxymethyl)benzene) prevailed, indicating that methanol protected the hydroxyl group in VA from being oxidized to VAld. Catalysts containing alternative transition metals (Mn, Co, Cu and Ag) supported on Al₂O₃ gave significantly lower activities compared to Ru/Al₂O₃ under identical reaction conditions. The Ru/Al₂O₃ catalyst was reused in three consecutive reaction runs in water, but a decrease in VAld yield was obtained after the third cycle possibly due to leaching of Ru from the support.
Co2 chemosorption by functionalized amino acid derivatives.
The absorption and desorption behaviour of carbon dioxide (CO2) using a composition comprising an ionic compound comprising a cation [A+] and an anion [B-] is described, wherein the anion [B-] is a mono-amine functionalized amino acid.
A Method for Effective Conversion of Saccharides to Furfural Compounds
The present invention relates to a method for the effective conversion of one or more mono-, di-, oligo- or polysaccharides to hydroxymethylfurfural (HMF), in an ionic liquid by means of a chromium catalyst mixture comprising chromium (II) and chromium (III) species. The invention also provides a catalyst mixture suitable for this conversion.

Aerobic oxidation of β-O-4 lignin model compounds with solid catalysts

Also registered as: WO2014EP64942, EP20130176259

COST Abstract MAYRA MELIAN.pdf

Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2015
Catalytic Alkylation of 2-Methylfuran with Formalin Using Supported Acidic Ionic Liquids

Biphasic alkylation of 2-methylfuran (2-MF) with formalin was carried out with a series of SBA-15 supported acidic ionic liquid catalysts (acidic SILCs) under mild reaction conditions. Acidic SILC with sulfonic acid groups (SO3H) and long alkyl chains was observed to have higher catalytic activity than commercial sulfonic acid resin catalysts for the alkylation reaction in terms of TONs/TOFs as well as selectivity (90%) toward the C11 oxygenate bis(5-methylfuran-2-yl)methane (BMFM). The reaction product was easily separated by addition of the nonpolar solvent n-heptane and additional water to form a biphasic system. The reactivity of other biomass-based substrates such as 3,4-dimethoxybenzaldehyde, furfural, glycolaldehyde, and glyceraldehyde was also investigated over acidic SILCs, and excellent yields of about 80% or higher were obtained of the corresponding condensed products (except from glyceraldehyde). Easy catalyst recovery from the aqueous phase after extraction of BMFM with n-heptane and reusability for at least five consecutive reaction runs without significant loss of catalyst activity was further exemplified for a selected catalyst.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, Guizhou University
Contributors: Li, H., Shunmugavel, S., Yang, S., Riisager, A.
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BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.45 SJR 1.657 SNIP 1.369
Web of Science (2017): Impact factor 6.14
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.92 SJR 1.572 SNIP 1.434
Web of Science (2016): Impact factor 5.951
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.39 SJR 1.389 SNIP 1.353
Web of Science (2015): Impact factor 5.267
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.3 SJR 1.218 SNIP 1.188
Web of Science (2014): Impact factor 4.642
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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Electronic versions:
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Research output: Research - peer-review › Journal article – Annual report year: 2015
Catalytic oxidation of lignin and lignin model compounds

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Melián Rodríguez, M., Shunmugavel, S., Kegnæs, S., Riisager, A.
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Catalytic oxidation of veratryl alcohol – a β-O-4 lignin model compound – to veratraldehyde

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
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Peer-reviewed: Yes
Electronic versions:
MAYRA_ABSTRACT_EuropaCat_Final.pdf
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Catalytic oxidation of veratryl alcohol – a β-O-4 lignin model compound – to veratraldehyde

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Melián Rodríguez, M., Shunmugavel, S., Kegnæs, S., Riisager, A.
Publication date: 2015
Peer-reviewed: Yes
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Europacat_poster_FINAL.pdf
Research output: Research - peer-review › Poster – Annual report year: 2015

CO2 adsorbers for upgrading of bio-gas to methan

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Schill, L., Riisager, A., Fehrmann, R.
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Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-31
Copper oxide as efficient catalyst for oxidative dehydrogenation of alcohols with air
The oxidative dehydrogenation of alcohols to carbonyl compounds was studied using CuO nanoparticle catalysts prepared by solution synthesis in buffered media. CuO nanoparticles synthesized in N-cyclohexyl-3-aminopropanesulfonic acid buffer showed high catalytic activity for the oxidation of benzylic, alicyclic and unsaturated alcohols to their corresponding carbonyl compounds with excellent selectivities. The observed trend in activity for conversion of substituted alcohols suggested a β-H elimination step to be involved, thus enabling a possible reaction mechanism for oxidative dehydrogenation of benzyl alcohols to be proposed. The use of CuO as an inexpensive and efficient heterogeneous catalyst under aerobic conditions provides a new noble metal-free and green reaction protocol for carbonyl compound synthesis.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, NanoChemistry
Contributors: Poreddy, R., Engelbrekt, C., Riisager, A.
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Deactivation of solid catalysts in liquid media: the case of leaching of active sites in biomass conversion reactions

This review is aimed to be a brief tutorial covering the deactivation of solid catalysts in the liquid phase, with specific focus on leaching, which can be especially helpful to researchers not familiarized with catalytic processes in the liquid phase. Leaching refers to the loss of active species from the solid that are transferred into the liquid medium, causing eventually a deactivation of the catalyst. Intriguingly, not many published studies have dealt with leaching, since this is a specific phenomenon in the liquid phase and heterogeneous catalysis is mainly carried out in gaseous phase. However, as a consequence of the development of new processes for biorefineries, an increasing number of reactions deal with liquid media, and thus, the stability and reusability of a solid catalyst in this situation represent a huge challenge that requires specific attention. Leaching of active phases is particularly problematic because of its irreversibility and it can be one of the main causes of catalyst deactivation in liquid media, threatening the sustainability of the process. This tutorial review presents a survey of the main aspects concerning the deactivation due to leaching of active species from the solid catalyst such as mechanisms, detection methods, impact of these factors on global activity and finally, some procedures to try and minimize the leaching or to cope with it. A decision flowchart is presented to help in the study of catalyst stability and reusability. Interesting biomass conversion reactions have been chosen as examples to illustrate the importance of these aspects.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, CSIC
Contributors: Sádaba, I., Lopez Granados, M., Riisager, A., Taarning, E.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Web of Science (2014): Impact factor 8.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
Web of Science (2013): Impact factor 6.852
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.64 SJR 2.444 SNIP 1.701
Web of Science (2012): Impact factor 6.828
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 6.46 SJR 2.32 SNIP 1.641
Web of Science (2011): Impact factor 6.32
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.142 SNIP 1.625
Web of Science (2010): Impact factor 5.472
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.088 SNIP 1.729
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.004 SNIP 1.544
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.131 SNIP 1.521
Web of Science (2007): Indexed yes
Heterogeneous catalysis in oxidation of lignin model compounds

General information
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Contributors: Melián Rodríguez, M., Shunmugavel, S., Kegnæs, S., Riisager, A.
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Peer-reviewed: Yes
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Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Heterogeneous catalysis in oxidation of lignin model compounds

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Melián Rodríguez, M., Shunmugavel, S., Kegnæs, S., Riisager, A.
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Peer-reviewed: No
Electronic versions:
  nordic.pdf
Research output: Research › Poster – Annual report year: 2014

Highly Selective Liquid-Phase Benzylation of Anisole with Solid-Acid Zeolite Catalysts
Zeolites were evaluated as solid acid catalysts for the liquid-phase benzylation of anisole with benzyl alcohol, benzyl bromide, and benzyl chloride at 80 °C. Among the examined zeolites, H-mordenite-10 (H-MOR-10) demonstrated particular high activity (>99 %) and excellent selectivity (>96 %) to the monobenzylated products, ortho/para benzyl anisole, using benzyl alcohol as reagent (anisole/alcohol molar ratio = 28). Analogous reactions with benzyl halides resulted in lower yields of the desired monobenzylated products. The conversion of benzyl alcohol was confirmed to be proportional to the amount of added H-MOR-10, and the linear free-energy relationship relating the conversion of substituted benzyl alcohol and substituent constants as well as the orientation effect of substituents of anisole on the distribution of ortho/para/meta isomers was evaluated.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Poreddy, R., Shunmugavel, S., Riisager, A.
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Peer-reviewed: Yes
Integration of CO₂ air capture and solid oxide electrolysis for methane production

This work studied the production of substitute natural gas (SNG) from CO₂ captured from the atmosphere followed by co-electrolysis with H₂O in solid oxide electrolyzer cells (SOEC) and downstream catalytic methane production. Over the coming 20 years, Denmark is on a track to remove fossil fuels from all sectors of the energy system except for transportation. In the recently published Energikoncept 2035 [1], the Danish grid operator, Energinet.dk, lays out a scenario based on 72% wind power and 21% biomass and waste in the electricity grid mix. In this scenario, biogas and electrolysis gasses are projected to be used for production of process heat, peak-load power generation and on the longer term to replace hydrocarbons in the most energy intensive parts of the transportation sector; especially aviation. As a prerequisite for the scenario, no biomass can be imported to enhance the supply of combustible resources. In such an energy system, technologies for production of CO₂ neutral hydrocarbons for easy storage and use in the existing infrastructure; especially in the natural gas grid; may be of great value. The studied technology fulfills those demands. The main goal of the work was to design a plant and develop a thermodynamic model of the plant operation, enabling analyses related to selection of operating parameters; analysis and optimization of internal heat recovery and integration between the main technological subsystems. Finally to identify the main areas of technological development through economic analyses. The work included experimental work on an example of a system for capture of CO₂: the humidity swing (HS) system, qualitatively evaluating the H₂O uptake and CO₂ desorption characteristics of the sorbent material, especially in relation to the supply of H₂O to the sorbent. It was found that H₂O supplied in the gas phase resulted in slow uptakes and desorption rates of CO₂ whereas supplying liquid water to the sorbent resulted in fast desorption in the first hours, after which the rate dropped sharply. A method was developed and used to characterize the impurities present in CO₂ stream from the HS system in addition to the temperature vacuum swing (TVS) system under development by Climeworks Ltd. The method relied on adsorption of impurities on a filter consisting of nickel-yttria-stabilized-zirconia (Ni/YSZ), similar to the material used in the fuel electrodes of SOECs followed by elemental analysis by glow discharge mass spectrometry. The method had a sub-ppm detection limit. Across the tested systems, a range of elements known to be detrimental to solid oxide cell (SOC) operation were detected in the range from tens of ppb to 20 ppm.

The SNG plant was modelled using the process integration software package PRO/II alongside the design process, and a series of minor studies using PRO/II and thermodynamic analysis software FactSage® aided the design process. This included studying a long range of questions such as alternative strategies for CO₂ compression; the structure of the methanation plant; and the risk of carbon formation in both SOEC and methanation reactors, etc. The model was based on a thermodynamic 0-dimensional model of the electrolyzer sub-system, developed to technological specifications from the thermodynamic SOEC model published by Sun et al. [2] This model was used for a study of operating parameters, and two design cases were identified for the full plant based on these results. The two cases both operated at 80 atm, and had SOEC operating temperatures of 850 °C and 600 °C. The area specific resistance (ASR) of the SOECs were extrapolated to high pressure and low temperatures based on data for standard DTU Energy Ni-YSZ based cells, and the pressure dependency of the individual cell processes. With the full plant model finished, the potential for internal recovery of surplus heat was analyzed, and a network of heat exchangers synthesized in order to minimize the requirements for external heating and cooling services. Based on the process flow sheets and the heat exchanger network, the dimensions and costs of the equipment of the plant were calculated and additional cost components such as installation of equipment, land use, labor costs, operation and maintenance, etc. were estimated according to standard methods. The plant had a yearly production capacity of 575,000 Nm³ of SNG with a methane content above 98.5% which resulted in a Wobbe index of 49 MJ/Nm³ which is sufficient for injection into the natural gas grid. The SOEC stack power was around 700 kW, and the plant operated a tan energy efficiency of 65% (HHV) and 58% (LHV). An economic analysis based on guidelines from the Danish energy agency and standard methods was conducted accounting for interest rates, taxes, depreciation etc. at a minimum...
acceptable rate of return set to the minimum of 4 %. The economic analysis resulted in SNG production prices of 1.88 €/Nm³ and 2.94 €/Nm³ based on an electricity price of 18.6 €/MJ, a price of process heat at 120 °C of 11.9 €/MJ and a price of cell area of 0.23 €/cm². The main cost drivers were identified as the capital costs of the SOEC and air capture systems and the heat exchanger network. For operating costs, the electricity price had a significant impact, whereas the dependency of the SNG price on the heat price was minor. The technical issues where discussed in separate chapters interspersed by chapters documenting the modelling and design process. Finally, a comprehensive discussion at the end treats the technical issues of the plant in the light of the economic analysis.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Ebbehej, S. L., Mogensen, M. B., Jensen, S. H., Riisager, A.
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**Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite**

Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH₂CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH₂DCOOD), when D₂O is introduced in the feed during the carbonylation reaction.

**General information**

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Web of Science (2016): Indexed yes
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Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite

Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH₂CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH₂DCOOD), when D₂O is introduced in the feed during the carbonylation reaction.

General information
State: Published
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
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BFI (2009): BFI-level 1
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Lignin Valorization by Heterogeneous Catalytic Oxidation

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Melián Rodríguez, M., Shunmugavel, S., Kegnæs, S., Riisager, A.
Publication date: 2015
Lignin Valorization using Heterogenous Catalytic Oxidation

The research interests in biomass conversion to fuels and chemicals has increased significantly in the last decade in view of current problems such as global warming, high oil prices, food crisis and other geopolitical scenarios. Many different reactions and processes to convert biomass into high-value products and fuels have been proposed in the literature, giving special attention to the conversion of lignocellulosic biomass, which does not compete with food resources and is widely available as a low cost feedstock. Lignocellulose biomass is a complex material composed of three main fractions: cellulose (40-50%), hemicellulose (25-35%) and lignin (20-30%). Lignin is mainly composed of three different monolignol monomers: p-coumaryl, coniferyl and sinapyl alcohol. These monomers are connected with various linkages with the most common one being the ß-O-4 linkage. The lignin structure is complex so different model compounds are often used to study lignin valorization. These model compounds contain the linkages present in lignin, simplifying catalytic analysis and present analytical challenges related to the study of the complicated lignin polymer and the plethora of products that could be obtained. Heiko Lange et al., has reported that the catalytic oxidation products of lignin and lignin model compounds range from aromatic aldehyde and carboxylic acid and they must be originate form oxidation of side chain. The products we obtained in these reactions are based on the severity of the reaction conditions. Here, we therefore present an overview of the recent research about conversion of some lignin model compounds using heterogeneous catalysis in oxidation reactions.

Mechanistic insights into the oxidative dehydrogenation of amines to nitriles in continuous flow

The oxidative dehydrogenation of various aliphatic amines to their corresponding nitrile compounds using RuO₂/Al₂O₃ catalysts in air was successfully applied to a continuous flow reaction. Conversions of amines (up to >99%) and yields of nitriles (up to 77%) varied depending on reaction conditions and the amine utilised. The presence of water was found to be important for the activity and stability of the RuO₂/Al₂O₃ catalyst. The Hammett relationship and in situ infrared spectroscopy were applied to divulge details about the catalytic mechanism of the oxidative dehydrogenation of amines over RuO₂/Al₂O₃ catalysts.
Xylose Isomerization with Zeolites in a Two-Step Alcohol–Water Process

Isomerization of xylose to xylulose was efficiently catalyzed by large-pore zeolites in a two-step methanol–water process that enhanced the product yield significantly. The reaction pathway involves xylose isomerization to xylulose, which, in part, subsequently reacts with methanol to form methyl xyluloside (step 1) followed by hydrolysis after water addition to form additional xylulose (step 2). NMR spectroscopy studies performed with 13C-labeled xylose confirmed the proposed reaction pathway. The most active catalyst examined was zeolite Y, which proved more active than zeolite beta, ZSM-5, and mordenite. The yield of xylulose obtained over H-USY (Si/Al=6) after 1 h of reaction at 1008°C was 39%. After water hydrolysis in the second reaction step, the yield increased to 47%. Results obtained from pyridine adsorption studies confirm that H-USY (6) is a catalyst that combines Brønsted and Lewis acid sites, and isomerizes xylose in alcohol media to form xylulose at low temperature. The applied zeolites are commercially available; do not contain any auxiliary tetravalent metals, for example, tin, titanium, or zirconium; isomerize xylose efficiently; are easy to regenerate; and are prone to recycling.
Absorption of Flue-Gas Components by Ionic Liquids

Gas separation by ionic liquids (ILs) is a promising new research field with several potential applications of industrial interest. Thus cleaning of industrial off gases seems to be attractive by use of ILs and Supported Ionic Liquid Phase (SILP) materials. The potential of selected ILs for absorption of NOX, CO2 and SO2 are demonstrated and the possible mechanism of absorption described on the molecular level. Special focus regards the interaction of the ILs with water vapor, which is an important feature in envisaged application of flue gas cleaning in power plants, waste incineration plants, cement and glass factories as well as on board ships.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Universite d'Aix-Marseille III
Contributors: Kolding, H., Thomassen, P. L., Mossin, S., Kegnaes, S., Riisager, A., Rogez, J., Mikaelian, G.
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BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.36 SJR 0.211 SNIP 0.244
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.36 SJR 0.212 SNIP 0.234
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.27 SJR 0.192 SNIP 0.231
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.29 SJR 0.241 SNIP 0.26
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.36 SJR 0.261 SNIP 0.28
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
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Acetalization of furfural with zeolites under benign reaction conditions

Acetalization is a viable method to protect carbonyl functionalities in organic compounds and offers a potential synthetic strategy for synthesizing derived chemicals. In this work, several families of commercial zeolites have been employed as solid acid catalysts in the acetalization of furfural to form furfural diethyl acetal at room temperature using ethanol as a renewable solvent. Among the tested catalysts, H-USY (6) provided the highest catalytic activity (79% acetal yield), excellent selectivity and reusability in five consecutive reaction runs. Process parameters such as, e.g. reaction time, catalyst loading and applicability of different lower alcohols were evaluated and optimized.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, University of Málaga
Contributors: Rubio-Caballero, J. M., Shunmugavel, S., Maireles-Torres, P., Riisager, A.
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Web of Science (2017): Impact factor 4.667
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.322 SNIP 1.369
Web of Science (2016): Impact factor 4.636
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4 SJR 1.335 SNIP 1.403
Web of Science (2015): Impact factor 4.312
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.72 SJR 1.315 SNIP 1.453
Web of Science (2014): Impact factor 3.893
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.39 SJR 1.299 SNIP 1.415
Web of Science (2013): Impact factor 3.309
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.38 SJR 1.469 SNIP 1.422
Web of Science (2012): Impact factor 2.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Amine-Functionalized Amino Acid-based Ionic Liquids as Efficient and High-Capacity Absorbents for CO2

Ionic liquids (ILs) comprised of ammonium cations and anions of naturally occurring amino acids containing an additional amine group (e.g., lysine, histidine, asparagine, and glutamine) were examined as high-capacity absorbents for CO2. An absorption capacity of 2.1 mol CO2 per mol of IL (3.5 mol CO2 per kg IL, 13.1 wt% CO2) was measured for [N66614][Lys] at ambient temperature and about 1 mol CO2 per mol of IL at 80°C (under 1 bar of CO2). This demonstrated that desorption is possible under CO2-rich conditions by temperature-swing absorption; three consecutive sorption cycles were performed with the IL. The mechanistic and kinetic study of the absorption process was further substantiated by NMR spectroscopy and in situ attenuated total reflectance FTIR for [N66614][Lys] and the homologous phosphonium-based IL [P66614][Lys]. This study revealed that carbamic acid was formed with CO2 in both ILs by chemisorption; however, the amino acid-carboxyl groups on the anion played an important—but different—catalytic role for the sorption kinetics in the two ILs. The origin of the cationic effect is speculated to be correlated with the strength of the ion interactions in the two ILs.
An improved method of preparation of nanoparticular metal oxide catalysts

The present invention concerns an improved method of preparation of nanoparticular vanadium oxide/anatase titania catalysts having a narrow particle size distribution. In particular, the invention concerns preparation of nanoparticular vanadium oxide/anatase titania catalyst precursors comprising combustible crystallization seeds upon which the catalyst metal oxide is coprecipitated with the carrier metal oxide, which crystallization seeds are removed by combustion in a final calcining step.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kristensen, S. B., Kunov-Kruse, A. J., Riisager, A., Fehrmann, R.
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Research output: Research › Patent – Annual report year: 2014

Catalytic Deoxygenation of Renewable Chemicals – Structure-Performance Studies

Generation of chemicals from a viable feedstock is an increasingly interesting field. One of the major issues is the high oxygen ratios in biomass. There are a multitude of ways to remove oxygen from organic molecules. This thesis deals with two topics: The dehydration of glucose into HMF and the decarbonylation of aldehydes both heterogeneous and in ionic liquids.

Chapter 1 provides a walkthrough of areas such as green chemistry, ionic liquids, biomass, dehydration of glucose in ionic liquids and decarbonylation. The topics are all taking into account the current research and is subjectively chosen to provide a broad platform for the following chapters. Furthermore, the objectives for the thesis are listed here.

Chapter 2 deals with the synthetic preparation of the catalysts and the catalytic setups.

Chapter 3 deals with the dehydration of glucose into HMF in ionic liquids. The system was investigated thoroughly via several spectroscopic techniques. This was done in order to obtain novel information in regard to the catalytically active sites. EXAFS results showed that during the catalytic reaction, a species of the form CrCl4O2 was formed from CrCl6 in the solution. These are the predominant chromium containing species in the solution. EPR results showed the presence of a S= 1/2 spin system, and the only possible choice is radical formation. Optical absorption spectroscopy showed a change in the ligand field around the chromium.

Chapter 3 also deals with the homogeneous decarbonylation of aldehydes. The investigation of the effects of the ionic liquids in the catalytically active species is investigated in depth and the system [Rh(dppp)2]Cl in BMImCl was shown to be the most active combination. The reusability of the system showed great potential. The system showed a potential to decarbonylate both aliphatic and aromatic aldehydes.

Finally Chapter 3 looks at the heterogeneous decarbonylation of aldehydes, focussing on a continuous flow setup. The catalytic effect of oxidation state and ligandsphere is investigated. And the effects of temperature, solvent and substrate were under scrutiny. The catalyst decomposition was pictured by the aid of TEM and the formation of nanoparticles explained.

Chapter 4 concerns the summation of the results as well as the future perspectives for the respective applications and scientific developments.

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Contributors: Malcho, P., Riisager, A.
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Catalytic routes from biomass to fuels
The carbon-based chemicals and fuels that are necessary to meet the energy demand for our society originate presently almost exclusively from inexpensive fossil resources – coal, oil and natural gas. The forecast of diminishing and more expensive petroleum reserves has, however, engaged the chemical industry to find new feasible chemocatalytic routes to convert the components of lignocellulosic plant biomass (green biomass) as well as aquatic biomass (blue biomass) into potential platform chemicals that can replace the fossil based chemicals in order to leave the chemical supply and value chain unaffected. This presentation will survey the status of biofuels production from different sources, and discuss the sustainability of making transportation fuels from biomass. Furthermore, recently developed chemocatalytic technologies that allow efficient conversion of lignocellulosic biomass components into transportation fuels and fuel additives will be highlighted.

Catalytic Synthesis of Nitriles in Continuous Flow
The objective of this thesis is to report the development of a new, alternative process for the flexible production of nitrile compounds in continuous flow. Nitriles are an important class of compounds that find applications as solvents, chemical intermediates and pharmaceutical compounds. The process reported here involves the oxidative dehydrogenation of amine compounds to their corresponding nitrile using air as the oxidant, water as the solvent where possible and solid RuO₂/Al₂O₃ catalysts. Chapter 1 begins by outlining the aims of this thesis and then gives a short, basic introduction to concepts and techniques that are important to the contents of this thesis. Furthermore, relevant literature is reviewed to support the choice of using RuO₂/Al₂O₃ catalysts and the oxidative dehydrogenation of amines for the desired new process for the production of nitriles. Chapter 2 describes a new, alternative path to acetonitrile from ethanol via the oxidative dehydrogenation of ethylamine. The catalytic activity and product ratios of the batch and continuous flow reactions are compared and the effect of reaction conditions on the reaction is investigated. The effects of ammonia in the reaction and of catalyst calcination are also explored. High conversions (up to 100 %) and selectivities (80-90 %) are reported using optimized reaction conditions. Chapter 3 includes details of in situ infrared spectroscopy experiments, observing the surface of the RuO₂/Al₂O₃ catalyst during calcination in air, oxidative dehydrogenation of ethylamine and post-reaction purging. Chapter 4 outlines the application of RuO₂/Al₂O₃ catalysts to the oxidative dehydrogenation of benzylamine in air, utilizing a new reaction setup. Again, batch and continuous flow reactions are compared and the effects of reaction conditions, ammonia presence and catalyst calcination are reported. Moderate benzonitrile yields (up to 62 %) and high conversions (up to 100 %) are reported. Chapter 5 describes the detailed characterization of RuO₂/Al₂O₃ catalysts and optimization of the catalyst ruthenium loading. Application of optimized RuO₂/Al₂O₃ catalysts to the oxidative dehydrogenation of benzylamine is described and increased benzonitrile yields are reported (up to 82 %). Chapter 6 reports the application of oxidative dehydrogenation of amines using air and RuO₂/Al₂O₃ catalysts to a range of substituted aromatic amines and longer chain aliphatic amines. Substituent groups of aromatic amines are found to affect both the rate of amine conversion and nitrile production. Novel attempts are made to apply the Hammett relationship to the oxidative dehydrogenation of amines using air and RuO₂/Al₂O₃ catalysts in continuous flow. The effect of the presence of water in the reaction is also investigated. Chapter 7 includes an overview of how the contents of this thesis attempt to cover the aims stated in Chapter 1 and suggests future improvements to be made to the nitrile production process.
Conversion of carbohydrates to levulinic acid esters

The present invention relates to the field of converting carbohydrates into levulinic acid, a platform chemical for many chemical end products. More specifically the invention relates to a method for converting carbohydrates such as mono-, di- or polysaccharides, obtained from for example biomass production into a suitable levulinic acid ester in the presence of a zeolite or zeotype catalyst and a suitable alcohol, and the ester may be further converted into levulinic acid if desired.

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Contributors: Shunmugavel, S., Riisager, A.
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Research output: Research › Patent – Annual report year: 2014

CO₂ sorption by supported amino acid ionic liquids

The present invention concerns the absorption and desorption behaviour of carbon dioxide (CO₂) using ionic liquids derived from amino acids adsorbed on porous carrier materials.

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Contributors: Fehrmann, R., Riisager, A., Kolding, H., Shunmugavel, S.
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Depolymerization of organosolv lignin using doped porous metal oxides in supercritical methanol

An isolated, solvent-extracted lignin from candlenut (Aleurites moluccana) biomass was subjected to catalytic depolymerization in the presence of supercritical methanol, using a range of porous metal oxides derived from hydrotalcite-like precursors. The most effective catalysts in terms of lignin conversion to methanol-soluble products, without char formation, were based on copper in combination with other dopants based on relatively earth-abundant metals. Nearly complete conversion of lignin to bio-oil composed of monomers and low-mass oligomers with high aromatic content was obtained in 6 h at 310 °C using a catalyst based on a Cu- and La-doped hydrotalcite-like precursor. Product mixtures were characterized by NMR spectroscopy, gel permeation chromatography, and GC-MS. © 2014.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Yale University
Contributors: Warner, G., Hansen, T. S., Riisager, A., Beach, E. S., Barta, K., Anastas, P. T.
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Direct catalytic transformation of carbohydrates into 5-ethoxymethylfurfural with acid–base bifunctional hybrid nanospheres

A series of acid–base bifunctional hybrid nanospheres prepared from the self-assembly of basic amino acids and phosphotungstic acid (HPA) with different molar ratios were employed as efficient and recyclable catalysts for synthesis of liquid biofuel 5-ethoxymethylfurfural (EMF) from various carbohydrates. A high EMF yield of 76.6%, 58.5%, 42.4%, and 36.5% could be achieved, when fructose, inulin, sorbose, and sucrose were used as starting materials, respectively. Although, the acid–base bifunctional nanocatalysts were inert for synthesis of EMF from glucose based carbohydrates, ethyl glucopyranoside in good yields could be obtained from glucose in ethanol. Moreover, the nanocatalyst functionalized with acid and basic sites was able to be reused several times with no significant loss in catalytic activity.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark, Guizhou University
Contributors: Li, H., Khokarale, S. G., Kotni, R., Shunmugavel, S., Riisager, A., Yang, S.
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Scopus rating (2016): CiteScore 6.04 SJR 2.232 SNIP 2.109
Web of Science (2016): Impact factor 5.589
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.24 SJR 2.023 SNIP 2.079
Web of Science (2015): Impact factor 4.801
Improvement of trans-sialylation versus hydrolysis activity of an engineered sialidase from Trypanosoma rangeli by use of co-solvents.

Biocatalytic trans-sialylation is relevant for the design of biomimetic oligosaccharides such as human milk oligosaccharides. t-Butanol and ionic liquids, EAN (ethylammonium nitrate), [MMIm][MeSO4] (1,3-dimethylimidazolium methyl sulfate), and [C2OHMIm][PF6] (1-(2-hydroxyethyl)-3-methylimidazolium hexafluorophosphate), were examined as
co-solvents for the improvement of the synthesis versus hydrolysis ratio in the trans-sialylation of lactose, catalysed by an engineered sialidase from Trypanosoma rangeli. The use of 25 % (v/v) t-butanol as co-solvent significantly increased 3'-sialyllactose production by 40 % from 1.04 ± 0.09 to 1.47 ± 0.01 mM. The synthesis versus hydrolysis ratio increased correspondingly by 1.2-times. 1-2.5 % (v/v) EAN or [C2OHMIm][PF6] improved the synthesis versus hydrolysis ratio up to 2.5-times but simultaneously decreased the 3'-sialyllactose yield, probably due to enzyme inactivation caused by the ionic liquid. [MMIm][MeSO4] had a detrimental effect on the trans-sialylation yield and on the ratio between synthesis and hydrolysis.

General information
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark
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Scopus rating (2017): CiteScore 1.88 SJR 0.621 SNIP 0.695
Web of Science (2017): Impact factor 1.846
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.89 SJR 0.628 SNIP 0.725
Web of Science (2016): Impact factor 1.73
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.66 SJR 0.598 SNIP 0.664
Web of Science (2015): Impact factor 1.639
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.75 SJR 0.636 SNIP 0.811
Web of Science (2014): Impact factor 1.591
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.03 SJR 0.723 SNIP 0.94
Web of Science (2013): Impact factor 1.736
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.03 SJR 0.748 SNIP 0.949
Web of Science (2012): Impact factor 1.853
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.97 SJR 0.725 SNIP 0.913
Web of Science (2011): Impact factor 1.683
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Ionic liquids as recyclable and separable reaction media in Rh-catalyzed decarbonylation of aromatic and aliphatic aldehydes

Ionic liquids (ILs) have been applied as recyclable reaction media in the decarbonylation of aldehydes in the presence of a rhodium-phosphine complex catalyst. The performance of several new catalytic systems based on imidazolium-based ILs and [Rh(dppp)2]Cl (dppp: 1,3-diphenylphosphinopropane) were excellent in the decarbonylation of both aromatic and aliphatic aldehydes providing >99 yield of benzenes and alkanes, respectively. The catalytic performance depended, however, strongly on the employed IL and its thermal stability. In addition, the ILs afforded good catalyst immobilization as well as a biphasic system with the product allowing recovery and reuse of the employed catalyst.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Malcho, P., Garcia-Suarez, E. J., Riisager, A.
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Isomerisation of C4-C6 aldoses with zeolites
The present invention relates to isomerization of C4-C6 aldoses to their corresponding C4-C6 ketoses. In particular, the invention concerns isomerization of C4-C6 aldoses over solid zeolite catalysts free of any metals other than aluminum, in the presence of suitable solvent(s) at suitable elevated temperatures. C6 and C5 aldose sugars such as glucose and xyllose, which are available in large amounts from biomass precursors, are isomerized to fructose and xylulose respectively, in a one or two-step process over inexpensive commercially available zeolite catalysts, containing aluminum as the only metal in the catalyst. The ketoses obtained are used as sweeteners in the food and/or brewery industry, or treated to obtain downstream platform chemicals such as lactic acid, HMF, levulinic acid, furfural, MMHB, and the like.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Shunmugavel, S.
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Lignin valorization using heterogeneous catalytic oxidation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Melián Rodríguez, M., Shunmugavel, S., Kegnæs, S., Riisager, A.
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Electronic versions:
Mayra_Biomass_SummerSchool_Poster.pdf
Research output: Research › Poster – Annual report year: 2014

Pd-catalyzed ethylene methoxycarbonylation with Brønsted acid ionic liquids as promoter and phase-separable reaction media
Brønsted acid ionic liquids (BAILs) were prepared and applied as combined acid promoters and reaction media in Pd–phosphine catalyzed methoxycarbonylation of ethylene to produce methyl propionate. The BAILs served as alternatives to common mineral acids required for the reaction, e.g. methanesulfonic acid or sulfuric acid, resulting in high catalytic activity and selectivity towards methyl propionate. In addition, the BAILs yielded a biphasic system with the product and provided stability to palladium intermediates avoiding the undesirable formation of palladium black after reaction. These special features enabled facile methyl propionate separation and recovery of the ionic liquid catalyst system, thus allowing its re-use up to 15 times without apparent loss of catalytic activity or selectivity.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Garcia-Suarez, E. J., Khokarale, S. G., Nguyen van Buu, O., Fehrmann, R., Riisager, A.
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Selective Oxidations using Nanostructured Heterogeneous Catalysts

The aim of this thesis is to investigate and develop new efficient methods to oxidise alcohols and amines using heterogeneous catalysts and either $O_2$ or $H_2O_2$ as oxidants. From an economic and environmental point of view, these oxidants are ideal, because they are cheap and readily available and because they produce $H_2O$ as the only by-product.

Chapter 1 gives a short introduction to basic concepts in heterogeneous catalysis and green chemistry. Furthermore, the chapter gives an overview of the most important strategies to synthesise functional nanostructured materials and highlights how detailed understanding of size, shape and structure can help in the development of new and more efficient heterogeneous catalysts. The chapter is not intended to give a complete survey, but rather to introduce some of the recent developments in the synthesis of nanostructured heterogeneous catalysts. Finally, the chapter focuses on the use of supported metal catalysts for the selective oxidation of alcohols, which are currently dominated by the platinum group metals. Chapter 2 deals with the most important methods to characterise heterogeneous catalysts, including X-ray powder diffraction, physisorption analysis and electron microscopy. In particular, the chapter gives an introduction to electron tomography, which makes it possible to visualise and analyse the detailed three-dimensional features of nanostructured heterogeneous catalysts. Chapter 3 deals with the surprisingly high catalytic activity of supported gold nanoparticles with...
particular emphasis on the nature of the active site and the requirements needed to be considered when designing new catalytic systems. Furthermore, the chapter describes some of the most important methods to synthesise small and disperse gold nanoparticles on different supports. Chapter 4 describes a novel method for the two-step synthesis of amides from alcohols and amines using Au/TiO₂ and base as catalysts. In the first step, a methyl ester is obtained by the gold-catalysed aerobic oxidation of the alcohol in methanol. Base is promoting this reaction. In the second step, the amine is added and the methyl ester undergoes base-catalysed aminolysis to give the desired amide. As the same base is used for both reactions, the synthesis could be performed in a convenient one-pot procedure. The oxidative coupling was applied to a number of different alcohols and amines to demonstrate the versatility of the reaction protocol to a broader range of substrates. Chapter 5 describes the investigation of different silver catalysts for the synthesis of imines from alcohols and amines. The reactions were performed at relatively mild conditions (100°C and atmospheric pressure) without any additives or co-catalysts and afforded the desired imines with high selectivity (up to 99%). The highest catalytic activity was obtained with 5 wt% Ag/Al₂O₃ in toluene with air as oxidant, although the reaction also occurred under inert atmosphere by releasing H₂ into the gas-phase. Chapter 6 gives a short introduction to zeolites and the important concept of shape selectivity. Furthermore, the chapter describes the different strategies that can be used to overcome diffusion limitations. Chapter 7 demonstrates that mesoporous titanium silicalite-1 prepared by carbontemplating is an efficient catalyst for oxidation of pyridines to pyridine N-oxides using aqueous H₂O₂ as oxidant. The chapter begins with an introduction to N-oxides and an outline of recent development in the synthesis of ordered titanosilicates with focus on the efforts to overcome diffusion limitations. Chapter 8 describes how the continuing technological developments in biomass processing have made bioethanol a promising platform molecule for the production of a variety of value-added chemicals. Furthermore, the chapter describes a simple and effective method to encapsulate gold nanoparticles into a MFI zeolite and demonstrate their remarkable stability, catalytic activity and selectivity for the gas-phase oxidation of bioethanol to acetaldehyde, which may become a favourable and green alternative to the ethylene route.

Silver nanoparticles supported on alumina—a highly efficient and selective nanocatalyst for imine reduction
Silver nanoparticles supported on alumina were prepared and tested in the catalytic reduction of various imines to primary and secondary amines and were shown to be exceptionally active and chemoselective. Furthermore, the catalytic activity of the prepared nanocatalyst was also tested in the synthesis of secondary amines from primary amines in a tandem reaction protocol (oxidation–amination–reduction) using air and molecular hydrogen as oxidizing and reducing agents, respectively. The reported synthesis is performed under mild reaction conditions, which complies with the demands of modern organic synthesis. Due to the mild reaction conditions and high conversion as well as high selectivity, we consider that the utilization of silver nanoparticles supported on alumina represents an attractive and environmentally friendly alternative to the current synthesis of N-alkyl amines.
Solvent engineering and other reaction design methods for favouring enzyme-catalysed synthesis

This thesis investigates different methods for improving reaction yields of enzyme-catalysed synthesis reactions. These methods include the use of non-conventional media such as ionic liquids (ILs) and organic solvents as main solvents or as co-solvents as well as the use of more classical reaction design methods, i.e. enzyme immobilization and the use of an enzymatic membrane reactor. Two different enzyme classes, namely feruloyl esterases (FAEs) and sialidases are employed.

Using sinapoylation of glycerol as a model reaction it was shown that both the IL anion nature and the FAE structure were important for FAE activity and stability in IL-buffer (15% v/v) systems. The quantum chemistry-based COSMO-RS method was applied for explaining the IL anion effect in terms of hydrogen bonding capacity. Furthermore, the usefulness of COSMO-RS and other thermodynamically based tools in solvent selection for FAE-catalysed acylation reactions was reviewed. FAE type A from Aspergillus niger and an FAE from a commercial preparation from Humicola insolens, Depol 740L, could not catalyse the esterification of arabinoose or xylose with hydroxycinnamates in IL-buffer systems or in surfactantless microemulsion. However, both FAEs catalysed the feruloylation and/or sinapoylation of solvent cation C2OHIMIm+, thus underlining the broad acceptor specificity of FAEs and their potential for future solvent reactions.

An engineered sialidase from Trypanosoma rangeli, Tr6, catalyses trans-sialylation but the yield is hampered by substrate and product hydrolysis. The formation of 3'-sialyllactose from lactose and casein glycomacropeptide was used as a model reaction. Addition of 20-25% (v/v) t-butanol improved the trans-sialylation yield 1.4-fold and the synthesis/hydrolysis ratio 1.2-fold. Using ILs as co-solvents, the synthesis/hydrolysis ratio was also improved, but the trans-sialylation yield decreased, probably due to destabilization of Tr6 caused by the ILs. Returning to the conventional aqueous medium, immobilization of Tr6 on magnetic nanoparticles improved the synthesis/hydrolysis ratio 2.1-fold and increased the biocatalytic productivity of 2.5-fold. However, the recyclability of the immobilized enzyme was low. Reusing Tr6 seven times in a membrane reactor increased the trans-sialylation yield on the limiting substrate 1.3-fold, emphasizing the importance of the continuous product removal. Furthermore, the biocatalytic productivity was increased more than 9-fold as a result of the enzyme recovery.

In conclusion, where the use of non-conventional media is required for catalysis, e.g. in the thermodynamically controlled FAE-catalysed esterification, careful selection of both solvent system and the FAE itself is required to obtain adequate reaction yields. In contrast, for Tr6 the most promising results were obtained when keeping the reaction in aqueous medium and employing other reaction design methods such as continuous product removal and enzyme immobilization.

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Supported Rh-phosphine complex catalysts for continuous gas-phase decarbonylation of aldehydes.
Heterogeneous silica supported rhodium-phosphine complex catalysts are employed for the first time in the catalytic decarbonylation of aldehydes in continuous gas-phase. The reaction protocol is exemplified for the decarbonylation of p-tolualdehyde to toluene and further extended to other aromatic and aliphatic aldehydes achieving excellent results in terms of both conversion and selectivity.
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BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.93 SJR 1.306 SNIP 0.904
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.85 SJR 1.229 SNIP 0.918
Web of Science (2016): Impact factor 4.029
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.1 SJR 1.302 SNIP 1.006
Web of Science (2015): Impact factor 4.177
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.06 SJR 1.389 SNIP 1.064
Web of Science (2014): Impact factor 4.197
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.07 SJR 1.441 SNIP 1.08
Web of Science (2013): Impact factor 4.097
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.79 SJR 1.364 SNIP 0.865
Web of Science (2012): Impact factor 3.806
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.68 SJR 1.163 SNIP 0.751
Web of Science (2011): Impact factor 3.838
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.002 SNIP 0.602
Web of Science (2010): Impact factor 3.647
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.766 SNIP 0.596
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Zeolite-catalyzed isomerization of tetroses in aqueous medium

The isomerization of erythrose (ERO) was studied in water over commercially available large-pore zeolites such as, e.g., H-Y, H-USY and H-beta. Among the employed zeolites, H-USY(6) was found to efficiently isomerize the sugar yielding 45% erythrulose (ERU), 42% ERO and 3% of the epimer threose (THO) (corresponding to the equilibrium mixture), i.e. total tetrose yield 90%, after reaction for 5-7 h at 120 °C. Changing the solvent from water to methanol decreased the yield of ERU markedly to 18%, and gave only a total yield of tetroses of 27% which is significantly lower than obtained in water. Hence, the results demonstrate water to be a preferred solvent compared to lower alcohols for zeolite-catalyzed tetrose isomerization, which is opposite to what previously have been found for analogous pentose and hexose isomerization. A reuse study revealed further that H-USY(6) could be applied in at least five reaction runs with essentially unchanged activity and without significant aluminium leaching from the catalyst. The use of benign reaction conditions and an industrially pertinent solid catalyst in combination with water establishes a new, green tetrose isomerization protocol.

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Contributors: Shunmugavel, S., Riisager, A.
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Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
Web of Science (2017): Impact factor 5.365
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Zwitterion enhanced performance in palladium-phosphine catalyzed ethylene methoxycarbonylation

Zwitterions were used for the first time as promoters in ethylene methoxycarbonylation for the production of methyl propionate. They were found to improve the catalytic performance of the Pd–phosphine system. The presence of zwitterions could contribute to stabilize transition states and active catalytic Pd intermediates. The beneficial effect of the zwitterions was found to be most pronounced, when low amount of a strong acid (MeSO3H) was used with respect to palladium (below 2 equiv.). Under these conditions, phosphine ligand alkylation and reaction vessel corrosion are also anticipated to be less severe.

*General information*

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Absorption and oxidation of NO in ionic liquids

The present invention concerns the absorption and in situ oxidation of nitric oxide (NO) in the presence of water and oxygen in ionic liquid compositions at ambient temperature.
An alternative pathway for production of acetonitrile: ruthenium catalysed aerobic dehydrogenation of ethylamine

The oxidative synthesis of acetonitrile from ethylamine was studied using a supported ruthenium catalyst. The reaction was conducted in both batch and flow processes and high conversions (over 85%) were achieved in both cases. Selectivity of both reactions was improved by optimisation of reaction conditions, achieving over 90% selectivity in the batch process and 80% selectivity in the continuous flow process. The use of a selective solid catalyst that utilises a feedstock that can be derived from biomass, dioxygen as the oxidant and water as the solvent represents a new, green route for the independent and efficient production of acetonitrile.
Brønsted acid ionic liquid catalyzed formation of pyruvaldehyde dimethylacetal from triose sugars

A series of sulfonic acid functionalized ionic liquids (SO₃H-ILs) have been synthesized, characterized and investigated as catalysts for the conversion of the triose sugars, 1,3-dihydroxyacetone (DHA) and glyceraldehyde (GLA), to pyruvaldehyde dimethylacetal (PADA) in methanol. Depending on the reaction conditions and the applied SO₃H-ILs a good yield of up to 52% of PADA was obtained. Under identical reaction conditions the derivative of PADA, 1,1,2,2-tetramethoxy propane (TMP), could be obtained in yields up to 49% using another SO₃H-IL.
Catalyst for the carboxylation of carbonylated compounds in the gas phase

The invention relates to a catalyst for the carboxylation of carbonylated compounds in the gas phase. Said catalyst consists of a metal complex which is active when the carboxylation is under reaction conditions and an organic salt, which is solid under normal conditions and liquid under reaction conditions, on the porous inert support material.

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Contributors: Zipp, A., Ruedinger, C., Fehrmann, R., Hanning, C. W., Riisager, A.
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Catalytic conversion of lignocellulosic biomass using copper doped porous metal oxides

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Yale University
Contributors: Katalin, B., Anastas, P. T., Beach, E. S., Warner, G., Hansen, T. S., Riisager, A.
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Scopus rating (2014): SJR 0.101 SNIP 0.013
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Catalytic Performance of Zeolite-Supported Vanadia in the Aerobic Oxidation of 5-hydroxymethylfurfural to 2,5-diformylfuran

The catalytic performance of zeolite-supported vanadia catalysts was examined for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-diformylfuran (DFF) in organic solvents such as N,N-dimethylformamide (DMF), methyl isobutyl ketone, toluene, trifluorotoluene, and DMSO. Catalysts based on the four different zeolite supports H-beta, H-Y, H-mordenite, and H-ZSM-5 with 1–10 wt% vanadia loading were prepared and characterized by nitrogen physisorption, X-ray powder diffraction, scanning electron microscopy, ammonia temperature-programmed desorption, Raman spectroscopy and UV/Vis spectrophotometry. The H-beta zeolite catalysts were found to contain highly dispersed vanadium oxide species at all loadings, and provided the highest reaction selectivity towards DFF and the lowest metal leaching of the examined systems. In particular, 1 wt % V₂O₅/H-beta was found to be a stable, recyclable, and non-leaching catalyst for the production of DFF under mild conditions in DMF as solvent, although with low DFF yield. To increase the yield, oxidation of HMF at elevated pressures was also investigated with this catalyst. Under optimized conditions, a reaction selectivity towards DFF of >99 % at 84 % HMF conversion was obtained, albeit with some contribution from lixiviated species to the total catalyst activity.

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.47 SJR 1.695 SNIP 0.925
Web of Science (2017): Impact factor 4.674
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
The renewable chemical building block 5-hydroxymethylfurfural (HMF) was oxidized to 2,5-diformylfuran by an oxidation system consisting of the radical 2,2,6,6-tetramethyl-piperidin-1-oxyl (TEMPO) and CuCl. The system was optimized by exploring several reaction conditions and by employing nitrogen containing promoters (NCPs) to obtain excellent yields. In acetonitrile a 95% DFF yield was obtained after 24h with ambient pressure of dioxygen at room temperature in the presence of different NCPs, which – to our knowledge – is the best result reported thus far for this reaction. The use of NCPs made it further possible to apply various traditional solvents, e.g. acetone, methanol and methyl isobutyl ketone for the reaction. Additionally, HMF was oxidized to 2,5-furandicarboxylic acid by a modified oxidation protocol consisting of CuCl and t-BuOOH. In all the reactions, mild conditions, including room temperature were employed.
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 4.48 SJR 1.237 SNIP 1.257
Web of Science (2017): Impact factor 4.521
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.202 SNIP 1.336
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.08 SJR 1.218 SNIP 1.427
Web of Science (2015): Impact factor 4.012
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.04 SJR 1.335 SNIP 1.602
Web of Science (2014): Impact factor 3.942
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.01 SJR 1.448 SNIP 1.554
Web of Science (2013): Impact factor 3.674
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.89 SJR 1.573 SNIP 1.641
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ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.15 SJR 1.727 SNIP 1.752
Web of Science (2011): Impact factor 3.903
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.786 SNIP 1.641
Web of Science (2010): Impact factor 3.384
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.784 SNIP 1.82
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.882 SNIP 1.783
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.857 SNIP 1.638
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.679 SNIP 1.528
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.696 SNIP 1.687
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.815 SNIP 1.986
Web of Science (2004): Indexed yes
Efficient Isomerization of Glucose to Fructose over Zeolites in Consecutive Reactions in Alcohol and Aqueous Media.

Isomerization reactions of glucose were catalyzed by different types of commercial zeolites in methanol and water in two reaction steps. The most active catalyst was zeolite Y, which was found to be more active than the zeolites beta, ZSM-5, and mordenite. The novel reaction pathway involves glucose isomerization to fructose and subsequent reaction with methanol to form methyl fructoside (step 1), followed by hydrolysis to re-form fructose after water addition (step 2). NMR analysis with (13)C-labeled sugars confirmed this reaction pathway. Conversion of glucose for 1 h at 120 °C with H-USY (Si/Al = 6) gave a remarkable 55% yield of fructose after the second reaction step. A main advantage of applying alcohol media and a catalyst that combines Brønsted and Lewis acid sites is that glucose is isomerized to fructose at low temperatures, while direct conversion to industrially important chemicals like alkyl levulinates is viable at higher temperatures.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Universidad Rey Juan Carlos
Contributors: Shunmugavel, S., Paniagua, M., Melero, J. A., Riisager, A.
Pages: 5246-5249
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Journal of the American Chemical Society
Volume: 135
Issue number: 14
ISSN (Print): 0002-7863
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 14.05 SJR 8.127 SNIP 2.641
Web of Science (2017): Impact factor 14.357
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.492 SNIP 2.596
Web of Science (2016): Impact factor 13.858
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 12.81 SJR 6.775 SNIP 2.63
Web of Science (2015): Impact factor 13.038
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.92 SJR 6.294 SNIP 2.587
Web of Science (2014): Impact factor 12.113
Mechanistic investigation of the one-pot formation of amides by oxidative coupling of alcohols with amines in methanol

The one-pot formation of amides by oxidative coupling of alcohols and amines via intermediate formation of methyl ester using supported gold and base as catalysts was studied using the Hammett methodology. Determining the relative reactivity of four different para-substituted benzyl alcohol derivatives showed that the first step of the reaction generates a partial positive charge in the benzylic position (i.e. by hydride abstraction), while the second step of the reaction builds up negative charge in the rate determining step. The aminolysis of the methyl ester intermediate was further investigated by
means of DFT/B3LYP. The transition state structures and energies were determined for both a concerted and a neutral two-step reaction mechanism. As expected, the base-promoted two-step mechanism was found to be the most energetically favourable and this reaction mechanism was used to construct a theoretical Hammett plot that was in good agreement with the one obtained experimentally.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Mielby, J. J., Riisager, A., Fristrup, P., Kegnæs, S.
Pages: 211-216
Publication date: 2013
Peer-reviewed: Yes

**Publication information**

Journal: Catalysis Today
Volume: 203
ISSN (Print): 0920-5861
Ratings:

BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.55 SJR 1.347 SNIP 1.329
Web of Science (2017): Impact factor 4.667
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.322 SNIP 1.369
Web of Science (2016): Impact factor 4.636
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4 SJR 1.335 SNIP 1.403
Web of Science (2015): Impact factor 4.312
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.72 SJR 1.315 SNIP 1.453
Web of Science (2014): Impact factor 3.893
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.39 SJR 1.299 SNIP 1.415
Web of Science (2013): Impact factor 3.309
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.38 SJR 1.469 SNIP 1.422
Web of Science (2012): Impact factor 2.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.34 SJR 1.472 SNIP 1.562
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.761 SNIP 1.449
Web of Science (2010): Impact factor 2.993
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Method for enhancing the thermal stability of ionic compounds
This invention relates to a method for enhancing the thermal stability of ionic compounds including ionic liquids, by immobilization on porous solid support materials having a pore diameter of between about 20-200 AA, wherein the solid support does not have a pore size of 90 AA.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Robin, R., Gabriela, G.
Publication date: 2013

Publication information
IPC: A61K9/14
Patent number: WO2013030299
Date: 31/08/2011
Original language: English
Electronic versions:
WO2013030299A1.pdf
Research output: Research – Annual report year: 2013

Method for filling a reactor with a catalyst
The invention relates to a method for filling a reactor with a catalyst for the carbonylation of carbonylated compounds in the gas phase. According to said method, a SILP catalyst is covered with a filling agent which is liquid under normal conditions and is volatile under carbonylation reaction conditions, and a thus-treated catalyst is introduced into the reactor and the reactor is sealed.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Zipp, A., Ruedinger, A., Fehrmann, R., Hanning, C. W., Riisager, A.
Publication date: 2013

Publication information
Purification of 5-hydroxymethylfurfural (hmf) by crystallization
This invention relates to an efficient procedure for purifying HMF by crystallization at low temperature from an organic solvent.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Contributors: Riisager, A., Jensen, J. S., Ståhlberg, T. J. B., Woodley, J.
Publication date: 2013

Publication information
Country: Denmark
IPC: C07D307
Patent number: WO2013024162
Date: 21/02/2013
Original language: English
Electronic versions:
WO2013024162A1.pdf

Bibliographical note
DTU reference number: 92579
Research output: Research › Patent – Annual report year: 2013

Revisiting the Brønsted acid catalysed hydrolysis kinetics of polymeric carbohydrates in ionic liquids by in situ ATR-FTIR spectroscopy
A new versatile method to measure rates and determine activation energies for the Brønsted acid catalysed hydrolysis of cellulose and cellobiose (and other polymeric carbohydrates) in ionic liquids is demonstrated by following the C–O stretching band of the glycoside bond with in situ ATR-FTIR. An activation energy in excellent agreement with the literature was determined for cellulose hydrolysis, whereas a distinctly lower activation energy was determined for cellobiose hydrolysis. The methodology also allowed to independently determine activation energies for the formation of 5-hydroxymethylfurfural in the systems

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Kunov-Kruse, A. J., Riisager, A., Shunmugavel, S., Berg, R. W., Kristensen, S. B., Fehrmann, R.
Pages: 2843-2848
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: Green Chemistry
Volume: 15
Issue number: 10
ISSN (Print): 1463-9262
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Separation of Flue Gas Components by SILP (Supported Ionic Liquid-Phase) Absorbers

Reversible absorption of the flue gas components CO2, NO, NO2 and SO2 has been tested for different ionic liquids (ILs) at different temperatures and flue gas compositions where porous, high surface area carriers have been applied as supports for the ionic liquids to obtain Supported Ionic Liquid-Phase (SILP) absorber materials. The use of solid SILP absorbers with selected ILs were found to significantly improve the absorption capacity and sorption dynamics at low flue gas concentration, thus making the applicability of ILs viable in technical, continuous flow processes for flue gas cleaning. The results show that CO2, NO and SO2 can be reversible and selective absorbed using different ILs and that Supported Ionic Liquid-Phase (SILP) absorbers are promising materials for industrial flue gas cleaning. Absorption/desorption dynamics can be tuned by temperature, pressure and gas concentration.

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General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 433-442
Publication date: 2013
Peer-reviewed: Yes

Publication information
Journal: E C S Transactions
Volume: 50
Issue number: 11
ISSN (Print): 1938-5862
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.36 SJR 0.211 SNIP 0.244
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.36 SJR 0.212 SNIP 0.234
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.27 SJR 0.192 SNIP 0.231
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.29 SJR 0.241 SNIP 0.26
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.36 SJR 0.261 SNIP 0.28
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Structural Characterization of 1,1,3,3-Tetramethylguanidinium Chloride Ionic Liquid by Reversible SO2 Gas Absorption

A unique new ionic liquid–gas adduct solid state compound formed between 1,1,3,3-tetramethylguanidinium chloride ([tmgH]Cl) and sulfur dioxide has been characterized by X-ray diffraction and Raman spectroscopy. The structure contains SO2 molecules of near normal structure kept at their positions by Cl−S interactions. The crystals belong in the orthorhombic system, space group Pbcn, with unit cell dimensions of a = 15.6908(10) Å, b = 9.3865(6) Å, and c = 14.1494(9) Å, angles α = β = γ = 90°, and Z = 8 at 120 K. The [tmgH]Cl has a very high absorption capacity of nearly 3 mol of SO2 per mol of [tmgH]Cl at 1 bar of SO2 and at room temperature. However, part of the absorbed SO2 was liberated during the crystallization, probably because the crystal only accommodates one molecule of SO2 per [tmgH]Cl. The nature of the high absorption capacity of [tmgH]Cl as well as of the homologous compounds with bromide and iodide are discussed. Some of these salts may prove useful as reversible absorbents of SO2 in industrial flue gases.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Centre for Catalysis and Sustainable Chemistry
Contributors: Berg, R. W., Harris, P., Riisager, A., Fehrmann, R.
Pages: 11364−11373
Publication date: 2013
Peer-reviewed: Yes

Publication information
Volume: 117
ISSN (Print): 1089-5639
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Zeolite Catalyzed Transformation of Carbohydrates to Alkyl Levulinates

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Riisager, A.
Pages: 1754-1757
Publication date: 2013
Peer-reviewed: Yes

**Publication information**
Journal: ChemCatChem
Volume: 5
Issue number: 7
ISSN (Print): 1867-3880
Acetic Acid Formation by Selective Aerobic Oxidation of Aqueous Ethanol over Heterogeneous Ruthenium Catalysts

Heterogeneous catalyst systems comprising ruthenium hydroxide supported on different carrier materials, titania, alumina, ceria, and spinel (MgAl2O4), were applied in selective aerobic oxidation ethanol to form acetic acid, an important bulk chemical and food ingredient. The catalysts were characterized by X-ray powder diffraction (XRPD), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), and nitrogen physisorption and utilized in the oxidation of 2.5–50 wt % aqueous ethanol solutions at elevated temperatures and pressures. The effects of Ru metal loading, pretreatment of catalysts, oxidant pressure, reaction temperature, and substrate concentration were investigated. Quantitative yield of acetic acid was obtained with 1.2 wt % Ru(OH)x/CeO2 under optimized conditions (150 °C, 10 bar O2, 12 h of reaction time, 0.23 mol % Ru to substrate).

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Electron Nanoscopy
Contributors: Gorbanev, Y., Kegnaes, S., Hanning, C. W., Hansen, T. W., Riisager, A.
Aerobic Oxidation of 5-(Hydroxymethyl)furfural in Ionic Liquids with Solid Ruthenium Hydroxide Catalysts

The aerobic oxidation of 5-(hydroxymethyl)furfural was investigated over solid ruthenium hydroxide catalysts in ionic liquids at elevated temperatures and pressures. Several different catalyst supports were tested in combination with various ionic liquids. The best result was obtained in [EMIm][OAc] at 100 °C with 30 bar of oxygen over Ru(OH) x /La2O3 which afforded 48 % of 2,5-furandicarboxylic acid and 12 % of 5-hydroxymethyl-2-furancarboxylic acid. During use the catalysts were found to leach some of the metal inventory. However, the leached Ru species did not contribute to the catalytic activity, thus verifying that the catalytic oxidation proceeded heterogeneously under the applied reaction conditions.

General information
Alkali resistivity of Cu based selective catalytic reduction catalysts: Potassium chloride aerosol exposure and activity measurements

The deactivation of V2O5–WO3–TiO2, Cu–HZSM5 and Cu–HMOR plate type monolithic catalysts was investigated when exposed to KCl aerosols in a bench-scale reactor. Fresh and exposed catalysts were characterized by selective catalytic reduction (SCR) activity measurements, scanning electron microscope–energy dispersive X-ray spectroscopy (SEM–EDX) and NH3-temperature programmed desorption (NH3-TPD). 95% deactivation was observed for the V2O5–WO3–TiO2 catalyst, while the Cu–HZSM5 and Cu–HMOR catalysts deactivated only 58% and 48%, respectively, after 1200 h KCl exposure. SEM analysis of the KCl aerosol exposed catalysts revealed that the potassium salt not only deposited on the catalyst surface, but also penetrated into the catalyst wall. Thus, the K/M ratio (M = V or Cu) was high on V2O5–WO3–TiO2 catalyst and comparatively less on Cu–HZSM5 and Cu–HMOR catalysts. NH3-TPD revealed that the KCl exposed Cu–HZSM5 and Cu–HMOR catalysts only experienced a slight loss of acidity while the V2O5–WO3–TiO2 catalyst lost most of the acidity. High alkali resistivity seems to be characteristic of the zeolite supported SCR catalysts which thus could be attractive for flue gas cleaning in biomass plants.
Alternative alkali resistant deNOx catalysts were prepared using three different supports ZrO$_2$, TiO$_2$ and Mordenite zeolite. The majority of the catalysts were prepared by incipient wetness impregnation of a commercial support, with vanadium, copper or iron precursor, one catalyst was prepared by one-pot sol–gel method. All catalysts were characterized by BET, XRPD and NH$_3$-TPD. Initial SCR activities of 8 out of 9 catalysts showed higher NO conversion at least at one temperature in the temperature range 300–500 °C compared to the conventional V$_2$O$_5$–WO$_3$/TiO$_2$ catalyst. After potassium poisoning (100–130 µmol of K/g of catalyst) the relative drop in SCR activity and acidity was lower for all the alternative catalysts compared to the industrial V$_2$O$_5$–WO$_3$/TiO$_2$ catalyst. Furthermore, Cu/MOR and Nano-V$_2$O$_5$/Sul-TiO$_2$ catalysts showed 8–16 times higher SCR activities than the conventional even after high potassium doping (250 and 280 µmol of K/g, respectively). The increased poisoning resistance was due to high substrate acidity (sulphated, heteropoly acid promoted and zeolite supports), substituting the active species of the catalyst (other than vanadium species, i.e. Cu, Fe) and new catalyst synthesis methods (Nano-V$_2$O$_5$/Sul-TiO$_2$ catalyst prepared by sol–gel method).

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Putluru, S. S. R., Kristensen, S. B., Due-Hansen, J., Riisager, A., Fehrmann, R.
Pages: 192-196
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Catalysis Today
Volume: 184
ISSN (Print): 0920-5861
Ratings:
  BFI (2019): BFI-level 1
  Web of Science (2019): Indexed yes
  BFI (2018): BFI-level 1
  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 1
  Scopus rating (2017): CiteScore 4.55 SJR 1.347 SNIP 1.329
  Web of Science (2017): Impact factor 4.667
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): CiteScore 4.26 SJR 1.322 SNIP 1.369
  Web of Science (2016): Impact factor 4.636
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 1
  Scopus rating (2015): CiteScore 4 SJR 1.335 SNIP 1.403
  Web of Science (2015): Impact factor 4.312
  BFI (2014): BFI-level 1
  Scopus rating (2014): CiteScore 3.72 SJR 1.315 SNIP 1.453
  Web of Science (2014): Impact factor 3.893
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 1
  Scopus rating (2013): CiteScore 3.39 SJR 1.299 SNIP 1.415
  Web of Science (2013): Impact factor 3.309
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): CiteScore 3.38 SJR 1.469 SNIP 1.422
  Web of Science (2012): Impact factor 2.98
  ISI indexed (2012): ISI indexed yes
Alternative potassium resistant deNOx catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2012
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Catalytic aerobic oxidation of bio-renewable chemicals
This thesis covers the investigation of new catalytic systems for the aerobic oxidation of chemicals derived from bio-renewable sources. The effects of different factors and conditions on the reactions were examined. The employed catalysts were characterized by physisorption measurements, SEM, TEM, EDS, XRF and other methods. Supported gold and ruthenium hydroxide catalyst systems were explored for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDA), a potential polymer building block for the plastic industry, or its dimethyl ester (FDMC). High product selectivities and yields were obtained under optimized conditions. Heterogeneous catalysts consisting of Au nanoparticles on different supports were shown to efficiently oxidize HMF to FDA or FDMC in water or methanol, respectively. Additionally, the reaction conditions were shown to be adjustable for the exclusive production of intermediate products of the oxidation. Catalysts consisting of Ru(OH)_x deposited on metal oxide
supports, such as, for instance, CeO$_2$ and MgAl$_2$O$_4$, were employed in the aerobic oxidation of HMF in different "green" reaction media, e.g. water and various ionic liquids, under base-free conditions. Moreover, a detailed study on the performance and stability of the ruthenium hydroxide catalysts on magnesium-containing supports under reaction conditions was conducted.

The aerobic oxidation of HMF to form another value-added chemical, 2,5-diformylfuran (DFF), was also investigated with supported Ru(OH)$_x$ catalysts in organic solvents. The examined catalyst systems and reaction conditions were also shown to be applicable for the efficient oxidation of other substituted furans. Furthermore, novel catalytic systems comprising vanadia supported on zeolites were investigated for the aerobic oxidation of HMF to DFF in organic solvents, and a lixiviation study was performed.

The oxidation of aliphatic alcohols over supported Ru(OH)$_x$ and RuO$_x$ catalysts is also described. The highly selective and efficient oxidation of ethanol to acetic acid was shown with supported Ru(OH)$_x$ and highly dispersed RuO$_x$, deposited on various metal oxides. Furthermore, this thesis presents the results of the catalytic aerobic oxidative degradation of higher alcohols over supported ruthenium hydroxide catalysts. A very efficient oxidative cleavage of vic-diols to form respective acids was also shown under examined conditions.

Thus, the oxidative transformations of biomass-derived chemicals over different gold and ruthenium-based catalyst systems with oxygen as the abundant oxidant were explored.

### General information

**State:** Published  
**Organisations:** Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Centre for Catalysis and Sustainable Chemistry  
**Contributors:** Gorbanev, Y., Woodley, J., Riisager, A.  
**Number of pages:** 300  
**Publication date:** 2012

**Publication information**  
**Place of publication:** Kgs. Lyngby  
**Publisher:** Technical University of Denmark (DTU)  
**Original language:** English  
**Electronic versions:** thesis_.PDF

**Research output:** Research › Ph.D. thesis – Annual report year: 2012

### Catalytic conversion of carbohydrates to alkyl levulinates with Brønsted acid ionic liquids

**General information**  
**State:** Published  
**Organisations:** Department of Chemistry, Centre for Catalysis and Sustainable Chemistry  
**Contributors:** Shunmugavel, S., Nguyen van Buu, O., Riisager, A.  
**Publication date:** 2012  
**Peer-reviewed:** Yes  
**Event:** Abstract from Green Solvents for Synthesis 2012, Boppard, Germany.  
**Research output:** Research - peer-review › Conference abstract for conference – Annual report year: 2013

### Catalytic conversion of glycolse to 5-hydroxymethylfurfural in ionic liquids: A techno-economic process assessment

**General information**  
**State:** Published  
**Organisations:** Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology  
**Contributors:** Riisager, A., Ståhlberg, T. J. B., Fu, W., Woodley, J.  
**Publication date:** 2012  
**Peer-reviewed:** Yes  
**Event:** Abstract from 243rd ACS National Meeting, San Diego, CA, United States.  
**Research output:** Research - peer-review › Conference abstract for conference – Annual report year: 2013

### Catalytic production of nitriles in batch and continuous flow systems

**General information**  
**State:** Published  
**Organisations:** Department of Chemistry, Centre for Catalysis and Sustainable Chemistry  
**Contributors:** Corker, E. C., Mentzel, U. V., Fehrmann, R., Riisager, A.  
**Publication date:** 2012  
**Peer-reviewed:** Yes
Characterization and parametrical study of Rh-TPPTS supported ionic liquid phase (SILP) catalysts for ethylene hydroformylation

The supported ionic liquid phase (SILP) catalysis technology was applied to continuous, gas-phase hydroformylation of ethylene. Rh-TPPTS SILP catalysts with relatively low ionic liquid loading were shown to be stable and highly active for ethylene hydroformylation. However, the catalytic activity, BET surface area and pore morphology of the catalysts depended on the content of ionic liquid. Hence, catalysts with high ionic liquid loading content showed deactivation at high reaction temperatures, possibly caused by redistribution of ionic liquid out of the pores under these conditions. (C) 2012 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Hanoi University of Science and Technology
Contributors: Hanh, N. T. H., Duc, D. T., Thang, V. D., Minh, T. L., Riisager, A., Fehrmann, R.
Pages: 136-141
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Catalysis Communications
Volume: 25
ISSN (Print): 1566-7367
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.45 SJR 0.929 SNIP 0.926
Web of Science (2017): Impact factor 3.463
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.33 SJR 0.914 SNIP 0.95
Web of Science (2016): Impact factor 3.33
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.55 SJR 0.98 SNIP 1.117
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.81 SJR 1.158 SNIP 1.314
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.6 SJR 1.201 SNIP 1.265
Web of Science (2013): Impact factor 3.32
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.2 SJR 1.163 SNIP 1.415
Web of Science (2012): Impact factor 2.915
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.51 SJR 1.251 SNIP 1.499
Web of Science (2011): Impact factor 2.986
CO2 capture technologies: current status and new directions using supported ionic liquid phase (SILP) absorbers

Current state-of-the-art techniques for CO2 capture are presented and discussed. Post-combustion capture of CO2 by absorption is the technology most easily retrofitted to existing installations, but at present this is not economically viable to install and run. Using ionic liquids instead of aqueous amine solutions overcomes the major thermodynamic issues. By applying SILP technology further advances, in terms of ease of handling and sorption dynamics, are obtained. Initial experimental studies showed that ionic liquids such as tetrahexylammonium prolinate, [N6666][Pro], provide a good candidate for CO2 absorption using SILP technology. Thus a solid SILP absorber comprised of 40 wt% [N6666][Pro] loaded on precalcined silica quantitatively takes up about 1.2 mole CO2 per mole of ionic liquid in consecutive absorption-desorption cycles in a flow-experiment performed with 0.09 bar of CO2 (9% CO2 in He).

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kolding, H., Fehrmann, R., Riisager, A.
Pages: 1648-1656
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Science China Chemistry
Volume: 55
Issue number: 8
ISSN (Print): 1674-7291
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
DeNOx of flue gases by ionic liquid gas absorbers

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Mossin, S. L., Riisager, A., Fehrmann, R.
Publication date: 2012
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2013

Original language: English
Keywords: CO2 capture, Absorption, Ionic liquids, SILP absorber
Source: dtu
Source-ID: n:oai:DTIC-ART:inspec/368022041::18784
Research output: Research - peer-review » Journal article – Annual report year: 2012
Efficient catalytic formation of furanic chemicals with ionic liquid technologies

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Riisager, A., Shunmugavel, S., Ståhlberg, T. J. B., Fristrup, P.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from EUCHEM 2012 Molten Salts and Ionic Liquids XXIV, Celtic Manor, Wales, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Enzymatic isomerization of glucose and xylose in ionic liquids
Glucose isomerase has been found for the first time to catalyze the isomerization of glucose to fructose in the ionic liquid N, N-dibutylethanolammonium octanoate (DBAO). Isomerization was achieved at temperatures of 60-80 degrees C although a substantial amount of mannose was formed at elevated temperatures via the Lobry-de Bruyn-van Ekenstein transformation. Complete recovery of the sugars after reaction was achieved by extraction with aqueous HCl, thus making the protocol attractive for continuous operation.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T. J. B., Woodley, J., Riisager, A.
Pages: 291-295
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Catalysis Science & Technology
Volume: 2
Issue number: 2
ISSN (Print): 2044-4753
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
Web of Science (2017): Impact factor 5.365
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.64 SJR 1.811 SNIP 1.287
Web of Science (2016): Impact factor 5.773
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.46 SJR 1.804 SNIP 1.314
Web of Science (2015): Impact factor 5.287
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.44 SJR 1.885 SNIP 1.47
Web of Science (2014): Impact factor 5.426
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.89 SJR 1.744 SNIP 1.296
Web of Science (2013): Impact factor 4.76
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.7 SJR 1.595 SNIP 1.036
Enzymkatalyseret syntese i ioniske væsker

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Zeuner, B., Riisager, A., Meyer, A. S.
Pages: 20-23
Publication date: 2012
Peer-reviewed: No

Publication information
Journal: Dansk Kemi
Volume: 93
Issue number: 3
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
URLs:
http://techmedia.swiflet.com/tm/dak/51/1/
Source: dtu
Source-ID: n:oai:DTIC-ART:dkart/341525486::25136
Research output: Research - peer-review > Journal article – Annual report year: 2012

Fast and accurate determination of the reaction kinetics of cellulose hydrolyse in ionic liquids using in-situ ATR-FTIR

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Riisager, A., Shunmugavel, S., Berg, R. W., Kristensen, S. B., Fehrmann, R.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from Green Solvents for Synthesis 2012, Boppard, Germany.
Research output: Research - peer-review > Conference abstract for conference – Annual report year: 2013

FDCA as a renewable substitute for TPS in polymers

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2012
Peer-reviewed: Yes
Gas-phase dehydration of acetic acid and NH3 to acetonitrile over zeolite H-ZSM-5

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Mentzel, U. V., Corker, E. C., Riisager, A., Fehrmann, R.
Number of pages: 2
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.
Electronic versions: atm_icc_aceticacid-amination-dehydration, res 2.doc

Bibliographical note
Poster presentation.

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Source: dtu
Source-ID: u::4516

Heterogenisation of Homogeneous Catalytic Processes by Supported Ionic Liquids Phase (SILP) Catalysis: A New Viable Technology for Industry

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Hanning, C. W., Kolding, H., Fehrmann, R.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.

Heteropoly acid promoted catalyst for SCR of NOx with ammonia
The present invention concerns the selective removal of nitrogen oxides (NOx) from gases. In particular, the invention concerns a process, a highly alkali metal resistant heteropoly acid promoted catalyst and the use of said catalyst for removal of NOx from exhaust or flue gases, said gases comprising alkali or earth alkali metals. Such gases comprise for example flue gases arising from the burning of biomass, combined biomass and fossil fuel, and from waste incineration units. The process comprises the selective catalytic reduction (SCR) of NOx, such as nitrogen dioxide (NO2) and nitrogen oxide (NO) with ammonia (NH3) or a nitrogen containing compound selected from ammonium salts, urea or a urea derivative or a solution thereof as a reductant.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Putluru, S. S. R., Riisager, A., Fehrmann, R.
Publication date: 2012

Publication information
Country: Denmark
IPC: B01D53/86
Patent number: WO2012028566
Date: 08/03/2012
Original language: English

Bibliographical note
DTU reference nummer: 92507-10
Research output: Research › Patent – Annual report year: 2012
Highly dispersed supported ruthenium oxide as an aerobic catalyst for acetic acid synthesis

The increasing need for shifting to renewable feedstocks in the chemical industry has driven research toward using green aerobic, selective oxidation reactions to produce bulk chemicals. Here, we report the use of a ruthenium mixed oxide/hydroxide (RuOx) on different support materials for the selective aerobic oxidation of ethanol to acetic acid. The RuOx was deposited onto different oxide supports using a new gas-phase reaction, which in all cases resulted in homogeneous nanoparticulate films. The RuOx particle size ranged from 0.3 to 1.5nm. The catalytic activity was evaluated on TiO2, Mg6Al2(CO3)(OH)16-4(H2O), MgAl2O4, Na2Ti6O13 nanotubes, ZnO, γ-Al2O3, WO3, CeO2, and Ce0.5Zr0.5O2 supports. The CeO2 supported RuOx had the highest activity, and selectivity toward acetic acid, of all the materials when normalized with respect to Ru-loading. This high activity was independent of the surface area of the support and the loading of RuOx under the tested conditions. This was attributed to the highly uniform size of the RuOx deposits, demonstrating that the deposition is suitable for producing small nanoparticles at high loadings. To elucidate the reason for the promotional effect of CeO2, Ce0.5Zr0.5O2 was investigated as a high oxygen storage capacity support, however, this did not result in higher catalytic activity. The high activity of CeO2 supports compared to the low activity ZnO appear correlated to the presence of high valence Ru(VI) species analogous to that observed in literature.

General information
State: Published
Organisations: Center for Individual Nanoparticle Functionality, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Chemistry, Center for Electron Nanoscopy, Centre for Catalysis and Sustainable Chemistry
Pages: 243-250
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Applied Catalysis A: General
Volume: 433-434
ISSN (Print): 0926-860X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.48 SJR 1.237 SNIP 1.257
Web of Science (2017): Impact factor 4.521
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.202 SNIP 1.336
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.08 SJR 1.218 SNIP 1.427
Web of Science (2015): Impact factor 4.012
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.04 SJR 1.335 SNIP 1.602
Web of Science (2014): Impact factor 3.942
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.01 SJR 1.448 SNIP 1.554
Web of Science (2013): Impact factor 3.674
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.89 SJR 1.573 SNIP 1.641
Web of Science (2012): Impact factor 3.41
In-situ Spectroscopic Determination of Catalytic Cellulose Depolymerization

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Fehrmann, R., Riisager, A.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.
Research output: Research - peer-review Conference abstract for conference – Annual report year: 2013

Ionic liquid-active pharmaceutical ingredients loaded on silica: Solids handling for liquid pharmaceutical forms

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Ionic liquids as reaction media with phase separation properties: Cation effect

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Sustainable and Green Chemistry
Contributors: Søndergaard, H., Sørensen, M. G., Riisager, A.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 5th Workshop on Fats and Oils as Renewable Feedstock for Chemical Industry, Karlsruhe, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Ionic liquids as solvents for catalytic decarbonylation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Sustainable and Green Chemistry
Contributors: Malcho, P., Fernandez Gomez, C., Riisager, A.
Publication date: 2012
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Ionic Liquids as Solvents for Catalytic Decarbonylation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Sustainable and Green Chemistry
Contributors: Malcho, P., Fernandez Gomez, C., Riisager, A.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Ionic liquids in integrated catalytic technologies to produce furanic chemical

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Organic Chemistry
Contributors: Riisager, A., Ståhlberg, T. J. B., Fu, W., Woodley, J., Fristrup, P.
Publication date: 2012
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Mordenite - Type Zeolite SCR Catalysts with Iron or Copper
Cu/mordenite catalysts were found to be highly active for the SCR of NO with NH3 and exhibited high resistance to alkali poisoning. Redox and acidic properties of Cu/mordenite were well preserved after poisoning with potassium unlike that of vanadium catalysts. Fe-mordenite catalysts also revealed much higher alkali resistivity than that of commercial V2O5/WO3-TiO2 (VWT) SCR catalyst which is currently used for NOx abatement in stationary installations. Unique support properties like high surface area and surface acidity, which are not available in the commercial VWT catalyst, seem to be essential requirements for the high alkali resistance. Mordenite-type zeolite based catalysts could therefore be attractive alternatives to conventional SCR catalysts for biomass fired power plant flue gas treatment.
New deNOx catalysts for biomass fired units

One-pot reduction of 5-hydroxymethylfurfural via hydrogen transfer from supercritical methanol

Catalytic conversion of HMF to valuable chemicals was achieved over a Cu-doped porous metal oxide in supercritical methanol. The hydrotalcite catalyst precursor is prepared following simple synthetic procedures, using inexpensive and earth-abundant starting materials in aqueous solutions. The hydrogen equivalents needed for the reductive deoxygenation of HMF originate from the solvent itself upon its reforming. Dimethylfuran, dimethyltetrahydrofuran and 2-hexanol were obtained in good yields. At milder reaction temperatures, a combined yield (DMF + DMTHF) of 58% was achieved. Notably, the formation of higher boiling side products and undesired char from HMF is not detected under these reaction conditions.
One-pot synthesis of amides by aerobic oxidative coupling of alcohols or aldehydes with amines using supported gold and base as catalysts
Synthesis of amides by aerobic oxidative coupling of alcohols or aldehydes with amines via intermediate formation of methyl esters is highly efficient and selective when using a catalytic system comprised of supported gold nanoparticles and added base in methanol.
Pharmaceutically active ionic liquids with solids handling, enhanced thermal stability, and fast release

Pharmaceutically active compounds in ionic liquid form immobilized onto mesoporous silica are stable, easily handled solids, with fast and complete release from the carrier material when placed into an aqueous environment. Depending on specific ion-surface interactions, they may also exhibit improved thermal stability when compared to the non-adsorbed compounds.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Vienna University of Technology, University of Santiago de Compostela, University of Alabama
Contributors: Bica, K., Rodríguez, H., Gurau, G., Andreea Cojocaru, O., Riisager, A., Fehrmann, R., Rogers, R. D.
Pages: 5422-5424
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Chemical Communications
Volume: 48
Issue number: 44
ISSN (Print): 1359-7345
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127
Process Design and Evaluation for Chemicals Based on Renewable Resources

One of the key steps in process design is choosing between alternative technologies, especially for processes producing bulk and commodity chemicals. Recently, driven by the increasing oil prices and diminishing reserves, the production of bulk and commodity chemicals from renewable feedstocks has gained considerable interest. Renewable feedstocks usually cannot be converted into fuels and chemicals with existing process facilities due to the molecular functionality and variety of the most common renewable feedstock (biomass). Therefore new types of catalytic methods as well as new types of processes for converting renewable feedstocks to bulk and commodity chemicals are required. In the future, it seems increasingly likely that a combination of biocatalysts (in the form of enzymes) as well as chemical catalysts will be needed in the production of bulk chemicals from renewable feedstocks. In addition, another characteristic of chemicals based on renewable feedstocks is that many alternative technologies and possible routes exist, resulting in many possible process flowsheets. The challenge for process engineers is then to choose between possible process routes and alternative technologies as well as to match different catalyst conditions. These kinds of problems are crucial, especially at the early stages of process development, when information is limited.

This thesis describes a methodological framework for dealing with the challenges and giving direction to research in the process development of chemicals based on renewable feedstocks. As an example, this thesis especially focuses on applying the methodology in process design and evaluation of the synthesis of 5-hydroxymethylfurfural (HMF) from the renewable feedstock glucose/fructose. The selected example is part of the chemoenzymatic process design of the synthesis 2,5-furandicarboxylic acid (FDA) from glucose.

By using the selected case study, the complexity and challenges for the process engineer to choose between different alternative routes and technologies as well as to combine two different kinds of catalysis (enzymatic catalysis and chemical catalysis) were illustrated.

Different process routes for the synthesis of HMF from fructose in the literature have been analyzed and evaluated. Using an aqueous route for HMF production is not economically feasible due to the low reaction yield. Using an anhydrous solvent for HMF synthesis is associated with high energy consumption and difficulties with solvent recycle in a large-scale production. The synthesis of HMF from fructose using a biphasic route is found to be promising, cost effective and give a better chance to be integrated with chemo-enzymatic cascades for producing FDA from glucose.

A process flowsheet using chemo-enzymatic cascades for HMF production from glucose has been proposed and evaluated. The process flowsheet is characterized by using glucose isomerase (EC 5.3.1.5) to convert glucose into fructose with a biphasic reaction for dehydration of fructose into HMF with recycle of the aqueous phase back to the enzymatic reaction. Costing analysis indicates the HMF production cost by the designed process is very sensitive to the dehydration reaction yield, the amount of solvent used in the whole process and the glucose price. In addition, increasing scale is also helpful to decrease the HMF production cost.

Using an ionic liquid (IL) route for HMF production has been evaluated with the dehydration reaction in [BMIm]Cl with different options starting from fructose and glucose with different initial concentrations. The HMF production cost is highly affected by the recycle of IL and catalyst. Processes with a high feed concentration show better economic potential than processes with a low feed concentration. IL processes starting from fructose are more costly than IL processes starting from glucose. High concentration feed of glucose showed the best economic potential.

To sum up, the dehydration reaction yield is found to be the key important factor to achieve a feasible production cost of HMF. The use of the organic solvent can not be avoided and plays a very important role in determining the process economics. Recycling (unconverted sugar, reaction medium and solvent) become essential issues for HMF processes to reach a feasible production cost. Future directions and suggestions for the synthesis of HMF from sugar in a large-scale have been proposed. The developed methodology is helpful in evaluation and giving research directions. The methodology can be applied to other chemical process design and evaluation problems and in particular those for the next generation of production processes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Fu, W., Woodley, J., Gani, R., Riisager, A.
Number of pages: 327
Publication date: 2012

Publication information
Publisher: Technical University of Denmark, Department of Chemical Engineering
Separation of flue gas components by ionic liquids: Fundamental chemistry and industrial application

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from Pacific Rim Meeting on Electrochemical and Solid-State Science, Honolulu, United States.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2013

Sn-Beta catalysed conversion of hemicellulosic sugars
Conversions of various pentoses and hexoses into methyl lactate has been demonstrated for the Sn-Beta catalyst. It is found that pentoses are converted to methyl lactate in slightly lower yields (~40%) than what is obtained for hexoses (~50%), but higher yields of glycolaldehyde dimethyl acetal are observed for the pentoses. This finding is in accordance to a reaction pathway that involves the retro aldol condensation of the sugars to form a triose and glycolaldehyde for the pentoses, and two trioses for hexoses. When reacting glycolaldehyde (formally a C2-sugar) in the presence of Sn-Beta, aldol condensation occurs, leading to the formation of methyl lactate, methyl vinylglycolate and methyl 2-hydroxy-4-methoxybutanoate. In contrast, when converting the sugars in water at low temperatures (100 °C), Sn-Beta catalyses the isomerisation of sugars (ketose–aldose epimers), rather than the formation of lactates.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, University of Wisconsin-Madison
Pages: 702-706
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Green Chemistry
Volume: 14
ISSN (Print): 1463-9262
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Solid acid catalysed formation of ethyl levulinate and ethyl glucopyranoside from mono- and disaccharides

Sulfonic acid functionalised SBA-15 (SO3H-SBA-15), sulfated zirconia and beta, Y, ZSM-5 and mordenite zeolite catalysts have been applied for the dehydration of sugars to ethyl levulinate and ethyl-D-glucopyranoside (EDGP) using ethanol as solvent and reactant. The SO3H-SBA-15 catalyst showed a high catalytic activity for the selective conversion of fructose to ethyl levulinate (57%) and glucose to EDGP (80%) at 140 °C, whereas the disaccharide sucrose yielded a significant amount of both products. The SO3H-SBA-15 catalysts were found to be highly active compared to the zeolites under identical reaction conditions.

Bibliographical note
Electronic supplementary information (ESI) available: Detailed HPLC analysis procedure, sugar isomerization distributions, carbon balances, NMR spectra and MS fragmentation patterns of key components. See DOI: 10.1039/c2gc16202d
Source: dtu
Source-ID: u::3536
Research output: Research - peer-review › Journal article – Annual report year: 2012
solid and catalyzed formation of ethyl levulinate from mono- and disaccharides

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Riisager, A.
Publication date: 2012
Peer-reviewed: Yes
Event: Abstract from 15th International Congress on Catalysis, Munich, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Supported Ionic Liquid Phase (SILP) Catalysis for the Production of Acetic acid by Methanol Carbonylation

The work presented here is focused on the development of a new reaction process. It applies Supported Ionic Liquid Phase (SILP) catalysis to a specific reaction. By reacting methanol and carbon monoxide over a rhodium catalyst, acetic acid can be formed. This reaction is important on a large scale industrially, with millions of tonnes of acetic acid being produced annually. Acetic acid is an important precursor for making adhesives, plastics and fabrics. By using the SILP concept we are able to carry out the reaction in a continuous system, allowing a steady production of acetic acid without having to stop and re-start the reaction. This sort of continuous flow reaction is a subject of great research effort in recent years as it is more sustainable (and in some cases financially viable) that the current method of carrying out chemical reactions in large size batch reactions.

The project started right at the beginning with the construction of a suitable test reactor, then followed by the synthesis and testing of all the catalysts reported.

A variety of nitrogen based ionic liquids were initially tested, giving good results and stability in the system. Later a number of phosphonium based salts were tested (these were no longer classified as ionic liquids due to melting points above 100°C). The phosphonium salts showed even better activity in the system compared to the ionic liquids.

Overall the work has shown that this process for the manufacture of acetic acid is viable industrially. This is backed up by the construction and operation of a pilot plant by Wacker Chemie AG in Munich.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Wacker Chemie AG
Contributors: Hanning, C. W., Fehrmann, R., Riisager, A.
Publication date: 2012

Publication information
Place of publication: Kgs.Lyngby
Publisher: DTU Chemistry
Original language: English
Electronic versions:
CHanning Thesis July 2012 Public.pdf
Source: dtu
Source-ID: u::4996
Research output: Research › Ph.D. thesis – Annual report year: 2012
Synergy effects in mixed Bi$_2$O$_3$, MoO$_3$ and V$_2$O$_5$ catalysts for selective oxidation of propylene

In this work, the possible synergy effects between Bi$_2$O$_3$, MoO$_3$ and V$_2$O$_5$, and between Bi$_2$Mo$_3$O$_{12}$ and BiVO$_4$, were investigated. The catalytic activity of the "mechanical mixture" of these compounds was measured. The mixture containing 36.96 mol% Bi$_2$O$_3$, 39.13 mol% MoO$_3$ and 23.91 mol% V$_2$O$_5$ (21.43 mol% Bi$_2$Mo$_3$O$_{12}$ and 78.57 mol% BiVO$_4$), corresponding to the compound Bi$_{1-x}$V$_{1-x}$Mo$_x$O$_4$ with $x = 0.45$ (Bi$_{0.85}$V$_{0.55}$Mo$_{0.45}$O$_4$), exhibited the highest activity for the selective oxidation of propylene to acrolein. The mixed sample prepared chemically by a sol–gel method possessed higher activity than that of mechanical mixtures.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Hanoi University of Science and Technology, Ghent University
Pages: 829-846
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Research on Chemical Intermediates
Volume: 38
Issue number: 3-5
ISSN (Print): 0922-6168
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.52 SJR 0.361 SNIP 0.563
Web of Science (2017): Impact factor 1.674
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.16 SJR 0.286 SNIP 0.464
Web of Science (2016): Impact factor 1.369
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.23 SJR 0.345 SNIP 0.71
Web of Science (2015): Impact factor 1.833
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.09 SJR 0.353 SNIP 0.534
Web of Science (2014): Impact factor 1.221
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.09 SJR 0.347 SNIP 0.638
Web of Science (2013): Impact factor 1.54
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.81 SJR 0.341 SNIP 0.465
Web of Science (2012): Impact factor 0.88
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.78 SJR 0.327 SNIP 0.327
Web of Science (2011): Impact factor 0.697
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.457 SNIP 0.563
Synthesis and Characterization of Ammonium-, Pyridinium-, and Pyrrolidinium-Based Sulfonamido Functionalized Ionic Liquids

New homologous ammonium-, pyridinium-, and pyrrolidinium-based sulfonamido functionalized ionic liquids have been synthesized in two steps using monoethanolamine, methanesulfonyl chloride, and tosyl chloride as precursors with ethanol as solvent. Attempts to synthesize dual amino functionalized ionic liquid containing both a primary and a secondary amine group in the same ionic liquid are also reported. All functionalized ionic liquids were characterized by 1H and 13C NMR. Melting point and thermal stability of the functionalized ionic liquids were measured by differential scanning calorimetry and thermogravimetric analysis.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Fehrmann, R., Riisager, A.
Pages: 3383-3394
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Synthetic Communications
Volume: 42
ISSN (Print): 0039-7911
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.15 SJR 0.328 SNIP 0.438
Web of Science (2017): Impact factor 1.377
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.09 SJR 0.352 SNIP 0.384
Web of Science (2016): Impact factor 1.134
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.06 SJR 0.357 SNIP 0.497
Web of Science (2015): Impact factor 1.065
BFI (2014): BFI-level 1
Thermodynamically based solvent design for enzymatic saccharide acylation with hydroxycinnamic acids in non-conventional media

Enzyme-catalyzed synthesis has been widely studied with lipases (EC 3.1.1.3), but feruloyl esterases (FAEs; EC 3.1.1.73) may provide advantages such as higher substrate affinity and regioselectivity in the synthesis of hydroxycinnamate saccharide esters. These compounds are interesting because of their amphiphilicity and antioxidative potential. Synthetic reactions using mono- or disaccharides as one of the substrates may moreover direct new routes for biomass upgrading in the biorefinery. The paper reviews the available data for enzymatic hydroxycinnamate saccharide ester synthesis in organic solvent systems as well as other enzymatic hydroxycinnamate acylations in ionic liquid systems. The choice of solvent system is highly decisive for enzyme stability, selectivity, and reaction yields in these synthesis reactions. To increase the understanding of the reaction environment and to facilitate solvent screening as a crucial part of the reaction design, the review explores the use of activity coefficient models for describing these systems and – more importantly – the use of group contribution model UNIFAC and quantum chemistry based COSMO-RS for thermodynamic predictions and preliminary solvent screening. Surfactant-free microemulsions of a hydrocarbon, a polar alcohol, and water are interesting solvent systems because they accommodate different substrate and product solubilities and maintain enzyme stability. Ionic liquids may provide advantages as solvents in terms of increased substrate and product solubility, higher reactivity and selectivity, as well as tunable physicochemical properties, but their design should be carefully considered in relation to enzyme stability. The treatise shows that thermodynamic modeling tools for solvent design provide a new toolbox to design enzyme-catalyzed synthetic reactions from biomass sources.
Absorption of gases in guanidinium based ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Minofar, B., Riisager, A., Fehrmann, R.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from First Ionic Liquid Symposium in Japan, Tottori, Japan.
Research output: Research - peer-review » Journal article – Annual report year: 2012

Activity and stability of feruloyl esterase A from Aspergillus niger in ionic liquid systems

Feruloyl esterases (FAEs; EC 3.1.1.73) are accessory plant cell wall-degrading enzymes, which catalyse the hydrolysis of the ester bond between ferulic acid and the monosaccharide to which it is covalently linked. FAEs can however also be brought to catalyse the (trans)esterification reaction in solvents that favour synthesis over hydrolysis, i.e. systems with low water content such as organic solvents or ionic liquids (ILs). The esterification of sinapic acid with glycerol catalysed by FAE A from Aspergillus niger (AnFaeA) in a series of ILs containing 15% (v/v) buffer showed that AnFaeA stability – and hence activity – was highly dependent on the anion nature: AnFaeA was stable and active for more than 2 hours in [PF6]--based ILs, but rapidly lost activity in [BF4]--based systems. This effect can be explained in terms of hydrogen bonding capacity of the two anions: As predicted by the quantum chemistry-based COSMO-RS method, [BF4]- has a tendency to form hydrogen bonds and thus interfere with the secondary structure of the enzyme, while [PF6]- is unlikely to form hydrogen bonds and therefore does not cause denaturation of the enzyme. Similar results have been obtained for lipases [1], but this is the first report on FAE stability in ILs [2]. COSMO-RS, which is now widely used for solvent screening in the complex IL systems [3], may be a valuable tool for fast enzyme stability predictions and/or solvent screening in the future.

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Zeuner, B., Riisager, A., Meyer, A. S.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 6th Danish Conference on Biotechnology and Molecular Biology, Vejle, Denmark.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2011

Aerobic oxidation of HMF to FDA with ruthenium containing ferrite-spinel catalyst

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Aerobic Oxidation of HMF to FDA with Ruthenium containing Ferrite-Spinel Catalyst

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Eyjolfsdottir, E., Riisager, A.
Publication date: 2011
Peer-reviewed: No
Event: Poster session presented at 10th EuropaCat Congress, Glasgow, United Kingdom.
Electronic versions:
prod11321618577207.europacat2011-final[1].pdf
URLs:
http://www.europacat.co.uk/

Bibliographical note
This work was supported by the Danish National Advanced Technology Foundation and Novozymes A/S.
Source: orbit
Source-ID: 313191
Research output: Research › Poster – Annual report year: 2011

Aerobic Oxidation Reactions with Highly Selective Gold Nanoparticle Catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Mielby, J. J., Kegnæs, S., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from The 22nd North American Catalysis Society Meeting, Detroit, United States.
Research output: Research › peer-review › Conference abstract for conference – Annual report year: 2011

Alkali resistant Cu/zeolite deNOx catalysts for flue gas cleaning in biomass fired applications

Cu/zeolite catalysts have been prepared by wet impregnation and characterized by N2 physisorption, EPR, H2-TPR and NH3-TPD methods. The Cu content was varied to optimize the loading as well as surface acidity. Optimized Cu/zeolite catalysts showed high surface acidity and excellent activity in the selective catalytic reduction (SCR) of NO with NH3. Furthermore, Cu/zeolite catalysts showed high SCR activity even after doping with potassium (0–500μmol/g) compared to a commercial vanadium catalyst which deactivated at lower potassium content. Fresh and deactivated catalysts were further examined to investigate the redox and acidic properties of the catalysts. The poisoning resistivity seems to be due to a combination of high surface area and strong acidity of the Cu/zeolite catalysts. The catalysts might be attractive alternatives to conventional catalysts for deNOx of flue gases from biomass fired power plants and other stationary industrial installations.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Putluru, S. S. R., Riisager, A., Fehrmann, R.
Pages: 183-188
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Applied Catalysis B: Environmental
Volume: 101
Issue number: 3-4
ISSN (Print): 0926-3373
Ratings:
BFI (2019): BFI-level 2
Alkali resistant Fe-zeolite catalysts for SCR of NO with NH3 in flue gases

Fe-zeolite catalysts were prepared by ionexchange and characterized by nitrogen physisorption, electron paramagnetic resonance (EPR) spectroscopy, NH3-temperature programmed desorption (TPD), H2-temperature programmed reduction (TPR) and Energy dispersive X-ray spectroscopy (EDX) methods. The effect of potassium doping on the acidic and redox properties of the Fe-zeolite catalysts were studied. The prepared catalysts showed high surface area and surface acidity. This is essential for increased alkali resistivity in comparison with conventional metal oxide supports like, e.g. TiO2 and ZrO2, towards e.g. potassium salts in flue gases from biomass fired power plants. These properties allowed both undoped and potassium doped Fe-zeolite catalysts to posses high activity during the selective catalytic reduction (SCR) of NO with NH3. The extent of deactivation of the Fe-zeolite catalysts was further compared with commercial V2O5–WO3–TiO2 catalyst (VWT) with various levels of potassium poisoning. While VWT catalysts severely deactivated at relative low potassium concentration levels the Fe-zeolite catalysts also showed superior alkali resistivity even at high potassium loadings.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, CHEC Research Centre, Department of Chemical and Biochemical Engineering
Contributors: Putluru, S. S. R., Jensen, A. D., Riisager, A., Fehrmann, R.
Pages: 1286-1292
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Topics in Catalysis
Volume: 54
ISSN (Print): 1022-5528
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.57 SJR 0.965 SNIP 0.753
Web of Science (2017): Impact factor 2.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.877
Web of Science (2016): Impact factor 2.486
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.41 SJR 0.926 SNIP 0.777
Web of Science (2015): Impact factor 2.355
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.29 SJR 0.987 SNIP 0.845
Web of Science (2014): Impact factor 2.365
Web of Science (2014): Indexed yes
Alternative Flue Gas Cleaning: Selective Gas Absorption by Ionic Liquids and by Supported Ionic Liquid-Phase (SILP) Absorbers

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Kegnæs, S., Due-Hansen, J., Abildstrøm, J. O., Riisager, A., Fehrmann, R.
Publication date: 2011
Peer-reviewed: Yes

Original language: English
Keywords: SCR of NO with ammonia, Fe-zeolite, Potassium poisoning, Deactivation

DOIs: 10.1007/s11244-011-9750-6
Source: orbit
Source-ID: 313189
Research output: Research - peer-review; Journal article – Annual report year: 2011
A method of producing hydroxymethylfurfural

The present invention relates to a method of producing 5-hydroxymethylfurfural by dehydration of fructose and/or glucose and/or mannose.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Publication date: 2011

Publication information
IPC: C07D307/46
Patent number: WO2011124639
Date: 13/10/2011
Priority date: 07/04/2010
Original language: English
Electronic versions:
WO2011124639A1.pdf
Research output: Research › Patent – Annual report year: 2011

Applying the COSMO model for the design of new ionic liquids for carbohydrate dissolution

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Riisager, A., Fehrmann, R.
Publication date: 2011
Peer-reviewed: Yes
Research output: Research › peer-review › Conference abstract for conference – Annual report year: 2011

Catalytic Conversion of Biomass in Ionic Liquids: Applying the COSMO Model for Designing the Solvents

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Riisager, A., Fehrmann, R.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Research output: Research › peer-review › Conference abstract for conference – Annual report year: 2011

Catalytic conversion of fructose to ethyl levulinate with Brønsted acid ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Nguyen van Buu, O., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Research output: Research › peer-review › Conference abstract for conference – Annual report year: 2011

Catalytic oxidation of unsaturated fatty esters in ionic liquids

General information
Challenges and perspectives for catalysis in production of diesel from biomass

The production of biofuels is expected to increase in the future due to environmental concerns, accelerating oil prices and the desire to achieve independence from mineral oil sources. Of the proposed methods for diesel production from biomass, the esterification and transesterification of plant oils or waste fats with methanol is the most prominent and has been applied industrially for a decade. Homogeneous acid and base catalysis is normally used, but solid acids, solid bases, ionic liquids and lipases are being developed as replacements. Hydrodeoxygenation of vegetable oils has likewise been commercialized. Diesel from biomass may also be produced by catalytic upgrading of bio-oils from flash pyrolysis, by aqueous-phase reforming of carbohydrates into non- or mono-functionalized hydrocarbons via consecutive reduction-condensation reactions, or by gasification of biomass to synthesis gas of CO and H2 and liquefaction to alkanes via Fischer-Tropsch synthesis. Here, the current challenges and perspectives regarding catalysis and raw materials for diesel production from biomass are surveyed. © Future Science Ltd.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Søndergaard, H., Fehrmann, R., Riisager, A.
Pages: 465-483
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Biofuels
Volume: 2
Issue number: 4
Conversion of Mono- and Disaccharides to Ethyl Levulinate and Ethyl Pyranoside with Sulfonic Acid-Functionalyzed Ionic Liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Nguyen van Buu, O., Riisager, A.
Pages: 723-726
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: ChemSusChem (Print)
Volume: 4
ISSN (Print): 1864-5631
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Impact factor 7.411
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Impact factor 7.226
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 7.33 SJR 2.53 SNIP 1.424
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 7.97 SJR 2.864 SNIP 1.663
Boric acid promotes the dehydration of glucose to 5-(hydroxy)methylfurfural in ionic liquids. Computational analyses by DFT calculations show a significant decrease in energy for the isomerization of glucose to fructose when the sugars are bound to boric acid and isotopic labeling NMR studies confirm that the mechanism proceeds via an ene–diol intermediate as described by A. Riisager, P. Fristrup et al. in their Full Paper on page 1456 ff.


General information
State: Published
Organisations: Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T. J. B., Rodriguez, S., Fristrup, P., Riisager, A.
Pages: 1369
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Chemistry: A European Journal
Volume: 17
Issue number: 5
ISSN (Print): 0947-6539
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.9 SJR 2.265 SNIP 1.02
Web of Science (2017): Impact factor 5.16
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.068
Web of Science (2016): Impact factor 5.317
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.99 SJR 2.461 SNIP 1.195
Web of Science (2015): Impact factor 5.771
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.51 SJR 2.526 SNIP 1.222
Web of Science (2014): Impact factor 5.731
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.68 SJR 2.643 SNIP 1.239
Web of Science (2013): Impact factor 5.696
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.55 SJR 2.935 SNIP 1.291
Web of Science (2012): Impact factor 5.831
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.46 SJR 2.902 SNIP 1.319
Web of Science (2011): Impact factor 5.925
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.791 SNIP 1.295
Web of Science (2010): Impact factor 5.476
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.753 SNIP 1.425
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.135 SNIP 1.473
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.449 SNIP 1.585
Scopus rating (2006): SJR 3.108 SNIP 1.553
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.78 SNIP 1.451
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.442 SNIP 1.483
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.365 SNIP 1.447
Dependency of the hydrogen bonding capacity of the solvent anion on the thermal stability of feruloyl esterases in ionic liquid systems

Three feruloyl esterases, EC 3.1.1.73, (FAEs), namely FAE A from Aspergillus niger (AnFaeA), FAE C from Aspergillus nidulans (AndFaeC), and the FAE activity in a commercial β-glucanase mixture from Humicola insolens (Ultraflo L) were tested for their ability to catalyse esterification of sinapic acid with glycerol in four ionic liquid (IL) systems. The IL systems were systematically composed of two selected pairs of cations and anions, respectively: [BMIm][PF6], [C2OHMIm][PF6], [BMIm][BF4], and [C2OHMIm][BF4]. AnFaeA had activity in [PF6]--based ILs, whereas the AndFaeC and the FAE in Ultraflo L had no appreciable activities and were generally unstable in the IL systems. FAE stability in the IL systems was apparently highly dependent on enzyme structure, and notably AnFaeA’s similarity to IL-compatible lipases may explain its stability. The thermal stability of AnFaeA was higher in buffer than in the IL systems, but at 40 °C and below there was no significant difference in AnFaeA stability between the buffer and the [PF6]--based systems: AnFaeA was stable in the [BMIm][PF6] and [C2OHMIm][PF6] systems for 2 h at 40 °C. However, the IL anion had a major effect on stability: [BF4]--caused rapid inactivation of AnFaeA, while [PF6]--did not. The cation did not have a similar effect. These observations could be explained in terms of the hydrogen bonding capacity of IL cations and anions via COSMO-RS simulations.

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 1550-1557
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Green Chemistry
Volume: 13
ISSN (Print): 1463-9262
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Effect of Support in Heterogeneous Ruthenium Catalysts Used for the Selective Aerobic Oxidation of HMF in Water

Heterogeneous ruthenium-based catalysts were applied in the selective, aerobic oxidation of 5-hydroxymethylfurfural, a versatile biomass-derived chemical, to form 2,5-furandicarboxylic acid. The oxidation reactions were performed in water with dioxygen as the oxidant at different pressures without added base. Catalysts were prepared by depositing catalytically active Ru(OH)x species on a number of different supports, such as titanium-, aluminum-, cerium-, zirconium-, magnesium- and lanthanum oxides, magnetite, spinel, hydrotalcite and hydroxyapatite. All the catalysts were found to be active in the oxidation reactions, and the choice of support was demonstrated to be important for the catalytic performance.

General information
State: Published
Heteropoly acid promoted Cu and Fe catalysts for the selective catalytic reduction of NO with ammonia

Cu/TiO2, Fe/TiO2 and heteropoly acid promoted Cu/TiO2, Fe/TiO2 catalysts were prepared and characterized by N2 physisorption, XRPD, NH3-TPD, H2-TPR and EPR. The catalysts exhibited only crystalline TiO2 phases with the active metals and promoters in highly dispersed state. The acidic properties were studied and compared with the catalytic activity for the selective catalytic reduction (SCR) of NO with ammonia. The SCR activities and acidity values of heteropoly acid promoted catalysts were found to be much higher than unpromoted catalysts. The influence of potassium poisons on the SCR activity and acidity was lower for promoted catalysts than for unpromoted catalysts. In the heteropoly acid promoted catalysts the SCR active Cu and Fe metals were protected from potassium poisons by bonding of the potassium to the Brønsted acid centres. Thus heteropoly acid promoted catalysts might be suitable for biomass fired power plant SCR applications.
Heteropoly acid promoted V2O5/TiO2 catalysts for NO abatement with ammonia in alkali containing flue gases

V2O5/TiO2 and heteropoly acid promoted V2O5/TiO2 catalysts were prepared and characterized by N2 physisorption, XRPD and NH3-TPD. The influence of the calcination temperature from 400 to 700°C on crystallinity and acidic properties was studied and compared with the activity for the selective catalytic reduction (SCR) of NO with ammonia. The SCR activity of heteropoly acid promoted catalysts was found to be much higher than for unpromoted catalysts. The stability of heteropoly acid promoted catalysts is dependent on calcination temperature and there is a gradual decrease in SCR activity and acidity with increase in calcination temperatures. Furthermore, the heteropoly acid promoted V2O5/TiO2 catalysts showed excellent alkali deactivation resistance and might therefore be alternative deNOx catalysts in biomass fired power plants.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, CHEC Research Centre, Department of Chemical and Biochemical Engineering
Contributors: Putluru, S. S. R., Jensen, A. D., Riisager, A., Fehrmann, R.
Pages: 631-637
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Catalysis Science & Technology
Volume: 1
ISSN (Print): 2044-4753
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
Web of Science (2017): Impact factor 5.365
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.64 SJR 1.811 SNIP 1.287
Web of Science (2016): Impact factor 5.773
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 5.46 SJR 1.804 SNIP 1.314
Web of Science (2015): Impact factor 5.287
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.44 SJR 1.885 SNIP 1.47
Web of Science (2014): Impact factor 5.426
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.89 SJR 1.744 SNIP 1.296
Web of Science (2013): Impact factor 4.76
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): CiteScore 3.7 SJR 1.595 SNIP 1.036
Web of Science (2012): Impact factor 3.753
ISI indexed (2012): ISI indexed no
Web of Science (2011): Impact factor
ISI indexed (2011): ISI indexed no
Original language: English
DOIs:
10.1039/c1cy00081k
High performance vanadia-anatase nanoparticle catalysts for the selective catalytic reduction of NO by ammonia

Highly active nanoparticle SCR deNO(x) catalysts composed of amorphous vanadia on crystalline anatase have been prepared by a sol-gel, co-precipitation method using decomposable crystallization seeds. The catalysts were characterized by means of XRPD, TEM/SEM, FT-IR, nitrogen physisorption and NH(3)-TPD. Due to the high-surface area anatase particles, loading of 20 wt% vanadia could be obtained without exceeding monolayer coverage of V(2)O(5). This resulted in unprecedented high deNO(x) SCR activity corresponding to a factor of two compared to an industrial reference and to other V(2)O(5)/TiO(2) catalysts reported in the literature in the examined temperature range of 200-400 degrees C. The catalysts showed very high resistivity towards potassium poisoning maintaining a 15-30 times higher activity than the equally poisoned industrial reference catalyst, upon impregnation by 280 mu mole potassium/g of catalyst. (C) 2011 Elsevier Inc. All rights reserved.
HMF oxidation with vanadia supported on zeolites: The search for a non-leaching catalyst

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Sádaba, I., Gorbaney, Y. Y., Putluru, S. S. R., López Granados, M., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from First International Congress on Catalysis for Biorefineries, Malaga, Spain.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2011

Hydrodeoxygenation of waste fat for diesel production: Study on model feed with Pt/alumina catalyst

Hydrodeoxygenation of waste fats and oils is a viable method for producing renewable diesel oil. In this study a model feed consisting of oleic acid and tripalmitin in molar ratio 1:3 was hydrotreated at 325°C with 20bars H2 in a stirred batch autoclave with a 5wt% Pt/γ-Al2O3 catalyst, and samples were extracted periodically and analyzed on GC. Despite the significant hydrogen pressure hydrogenation of both reactants were limited and decarboxylation or decarbonylation of the ester and carboxylic acid functionalities were highly favored, yielding carbon chain lengths of odd numbers. Moreover, Pd/γ-Al2O3 was observed to be slightly more active than Pt/γ-Al2O3 and had a higher ratio of decarboxylation and
decarbonylation to hydrogenation, while Ni/γ-Al2O3 was substantially less active than Pt and also showed a markedly lower ratio of decarboxylation and decarbonylation to hydrogenation. Variation of the temperature showed that triglycerides as well as free fatty acids were converted at all investigated temperatures, but the conversion of oleic acid increased from 6% to 100% when the temperature was increased from 250°C to 325°C. The tripalmitin reacted via a palmitic acid intermediate, and its conversion was limited by formation of this free fatty acid.
Ionic liquid Catalysis for Upgrading Biomass to Value-added Chemicals

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology
Contributors: Riisager, A., Ståhlberg, T. J. B., Shunmugavel, S., Fristrup, P., Fu, W., Woodley, J.
Publication date: 2011
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2011

Ionic Liquid Gas Absorption of Pollutants in Flue Gases

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Due-Hansen, J., Kegnæs, S., Godiksen, S., Riisager, A., Fehrmann, R.
Publication date: 2011
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2011

Ionic liquid mediated oxidation of unsaturated fatty esters

General information
State: Published
Ionic liquids as reaction media for transfer hydrogenation of epoxides

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Søndergaard, H., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Ionic liquids as solvent for transfer hydrogenation of epoxides

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Søndergaard, H., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Magnesium and nickel(II) furan-2,5-dicarboxylate

The salts hexaaquamagnesium furan-2,5-dicarboxylate, [Mg(H2O)(6)](C6H2O5), (I), and hexaaquanickel furan-2,5-dicarboxylate, [Ni(H2O)(6)](C6H2O5), (II), provide the first crystallographic characterization of the furan-2,5-dicarboxylate dianion. Both structures exhibit extensive three-dimensional hydrogen-bonding networks between the octahedral coordinated hexaaquametal(II) ions and the dicarboxylate anions. Although the two structures are not isomorphous, they contain essentially identical two-dimensional slabs. The distinction between the structures is that these slabs are related by translation in (II), whereas adjacent slabs in (I) are reflected relative to each other by the action of a glide plane. The reflection occurs so that the local contacts between slabs are not changed, and thus the hydrogen-bond networks are identical except for the orientation of the water molecules at the interface between slabs.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, University of Copenhagen
Contributors: Schau-Magnussen, M., Gorbanev, Y., Kegnæs, S., Riisager, A.
Pages: M327-M330
Publication date: 2011
Peer-reviewed: Yes

**Publication information**
Journal: Acta Crystallographica. Section C: Crystal Structure Communications
Volume: 67
ISSN (Print): 0108-2701
Ratings:
Web of Science (2019): Indexed yes
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 2.55 SJR 0.834 SNIP 1.213
Web of Science (2017): Impact factor 8.678
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.17 SJR 0.954 SNIP 1.579
Web of Science (2016): Impact factor 4.099
BFI (2015): BFI-level 1
Metal-Free Dehydration of Glucose to 5-(Hydroxymethyl)furfural in Ionic Liquids with Boric Acid as a Promoter

The dehydration of glucose and other hexose carbohydrates to 5-(hydroxymethyl)furfural (HMF) was investigated in imidazolium-based ionic liquids with boric acid as a promoter. A yield of up to 42% from glucose and as much as 66% from sucrose was obtained. The yield of HMF decreased as the concentration of boric acid exceeded one equivalent, most likely as a consequence of stronger fructose–borate chelate complexes being formed. Computational modeling with DFT calculations confirmed that the formation of 1:1 glucose–borate complexes facilitated the conversion pathway from glucose...
to fructose. Deuterium-labeling studies elucidated that the isomerization proceeded via an ene–diol mechanism, which is different to that of the enzyme-catalyzed isomerization of glucose to fructose. The introduced non-metal system containing boric acid provides a new direction in the search for catalyst systems allowing efficient HMF formation from biorenewable sources.

**General information**

State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T., Rodriguez, S., Fristrup, P., Riisager, A.
Pages: 1456-1464
Publication date: 2011
Peer-reviewed: Yes

**Publication information**

Journal: Chemistry: A European Journal
Volume: 17
Issue number: 5
ISSN (Print): 0947-6539
Ratings:
- BFI (2019): BFI-level 2
- Web of Science (2019): Indexed yes
- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 4.9 SJR 2.265 SNIP 1.02
- Web of Science (2017): Impact factor 5.16
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.068
- Web of Science (2016): Impact factor 5.317
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 4.99 SJR 2.461 SNIP 1.195
- Web of Science (2015): Impact factor 5.771
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): CiteScore 5.51 SJR 2.526 SNIP 1.222
- Web of Science (2014): Impact factor 5.731
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): CiteScore 5.68 SJR 2.643 SNIP 1.239
- Web of Science (2013): Impact factor 5.696
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): CiteScore 5.55 SJR 2.935 SNIP 1.291
- Web of Science (2012): Impact factor 5.831
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): CiteScore 5.46 SJR 2.902 SNIP 1.319
- Web of Science (2011): Impact factor 5.925
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.791 SNIP 1.295
- Web of Science (2010): Impact factor 5.476
New catalytic solutions for valorization of biomass resources

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 24th QUILL Lecture, Belfast, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

New Catalytic Systems with Ionic Liquids as Reaction Media for the Synthesis of Renewable Chemicals

General information
State: Published
Organisations: Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T., Riisager, A.
Publication date: 2011

Publication information
Place of publication: Kgs. Lyngby, Denmark
Publisher: Technical University of Denmark (DTU)
Original language: English
Electronic versions:
Tim Ståhlberg.pdf
Source: orbit
Source-ID: 281165
Research output: Research › Ph.D. thesis – Annual report year: 2012
New solutions in sustainable chemistry with advanced materials and catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from Research seminar at Carlsberg Laboratories, Copenhagen, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Novel deNOx catalysts for biomass fired units

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Sustainable and Green Chemistry
Contributors: Putluru, S. S. R., Fehrmann, R., Riisager, A., Due-Hansen, J., Kristensen, S. B.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

One-pot synthesis of amides by aerobic oxidative coupling of alcohols and amines using supported gold and base as catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Mielby, J. J., Kegnæs, S., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Oxidation of unsaturated fatty acids derivatives in ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Sørensen, M. G., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Palladium catalyst system comprising zwitterion and/or acid-functionalized ionic liquid
The present invention concerns a catalyst system in particular a catalyst system comprising Palladium (Pd), a zwitterion and/or an acid-functionalized ionic liquid, and one or more phosphine ligands, wherein the Pd catalyst can be provided by a complex precursor, such as Pd(CH3COO)2, PdCl2, Pd(CH3COCHCOCH3), Pd(CF3COO)2, Pd(PPh3)4 or Pd2(dibenzyldieneacetone)3. Such catalyst systems can be used for e.g. alkoxy carbonylation reactions, carboxylation reactions, and/or in a co-polymerization reaction, e.g. in the production of methyl propionate and/or propanoic acid, optionally in processes forming methyl methacrylate and/or methacrylic acid. Catalyst systems according to the invention are suitable for reactions forming separable product and catalyst phases and supported ionic liquid phase SILP applications.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Palladium catalyst system comprising zwitterion and/or acid-functionalized ionic liquid
The present invention concerns a catalyst system in particular a catalyst system comprising Palladium (Pd), a zwitterion and/or an acid-functionalized ionic liquid, and one or more phosphine ligands, wherein the Pd catalyst can be provided by a complex precursor, such as Pd(CH3COO)2, PdCl2, Pd(CH3COCHCOCH3), Pd(CF3COO)2, Pd(PPh3)4 or Pd2(dibenzylideneacetone)3. Such catalyst systems can be used for e.g. alkoxycarbonylation reactions, carboxylation reactions, and/or in a co-polymerization reaction, e.g. in the production of methyl propionate and/or propanoic acid, optionally in processes forming methyl methacrylate and/or methacrylic acid. Catalyst systems according to the invention are suitable for reactions forming separable product and catalyst phases and supported ionic liquid phase SILP applications.
Selective Aerobic Oxidation of 5-Hydroxymethylfurfural in Water Over Solid Ruthenium Hydroxide Catalysts with Magnesium-Based Supports

Solid catalyst systems comprised of ruthenium hydroxide supported on magnesium-based carrier materials (spinel, magnesium oxide and hydrotalcite) were investigated for the selective, aqueous aerobic oxidation of the biomass-derived chemical 5-hydroxymethylfurfural into 2,5-furandicarboxylic acid (FDA), a possible plastics precursor. The novel catalyst systems were characterized by nitrogen physisorption, XRPD, TEM and EDS analysis, and applied for the oxidation with no added base at moderate to high pressures of dioxygen and elevated temperatures. The effects of support, temperature and oxidant pressure were studied and optimized to allow a quantitative yield of FDA to be obtained.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Gorbanev, Y., Kegnæs, S., Riisager, A.
Pages: 1752-1760
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Catalysis Letters
Volume: 141
Issue number: 12
ISSN (Print): 1011-372X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.43 SJR 0.73 SNIP 0.729
Web of Science (2017): Impact factor 2.911
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.755 SNIP 0.786
Web of Science (2016): Impact factor 2.799
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.27 SJR 0.748 SNIP 0.749
Web of Science (2015): Impact factor 2.294
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.56 SJR 0.89 SNIP 0.928
Web of Science (2014): Impact factor 2.307
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.45 SJR 0.888 SNIP 0.931
Web of Science (2013): Impact factor 2.291
ISI indexed (2013): ISI indexed yes
Selective oxidation of propylene to acrolein by silica-supported bismuth molybdate catalysts

Silica-supported bismuth molybdate catalysts have been prepared by impregnation, structurally characterized and examined as improved catalysts for the selective oxidation of propylene to acrolein. Catalysts with a wide range of loadings (from 10 to 90 wt%) of beta bismuth molybdate (\(\beta\)-Bi\(_2\)Mo\(_2\)O\(_9\)) were studied to provide a better understanding about the distribution of active sites, and to elucidate the role of lattice oxygen in the reaction. The catalyst containing 50 wt% of beta bismuth molybdate on SiO\(_2\) was found to possess good distribution of active sites and sufficiently high lattice oxygen, which resulted in an extraordinary increase of the catalytic activity.
SILP Catalysis: The future of large scale ionic liquid catalysis?

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hanning, C. W., Nguyen van Buu, O., Riisager, A., Fehrmann, R.
Publication date: 2011
Peer-reviewed: Yes
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Structural characterization and catalytic properties of bis(1,1,3,3-tetramethylguanidinium) dichromate
The structure of bis(1,1,3,3-tetramethylguanidinium) dichromate was determined from powder X-ray diffraction data. The compound crystallizes in the monoclinic system (space group P21/n) with a = 10.79714 (15) Å, b = 11.75844 (16) Å, c = 8.15097 (11) Å, β = 109.5248 (6)°. The structure consists of dichromate anions (Cr2O72-) stabilized by tetramethylguanidinium cations ([H2NC(N(CH3)2)2]+ or [TMGH]+). Phase transitions of [TMGH]2Cr2O7 were determined by differential scanning calorimetry, thermal gravimetric analysis and in situ Raman spectroscopy, where the decomposition of the matrix into CrOX was found at 171-172°C. Further heat treatment to above 400°C resulted in formation of the thermodynamically stable Cr2O3, most likely with the [TMGH]+ cation as reductant. The catalytic activity of [TMGH]2Cr2O7 supported on TiO2 anatase in the selective catalytic reduction (SCR) of nitrogen oxide was also investigated, however only moderate activity was observed in the temperature range 100-400°C compared to the activity of e.g. vanadia supported on titania.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Centre for Catalysis and Sustainable Chemistry, University of Patras
Contributors: Due-Hansen, J., Ståhl, K., Boghosian, S., Riisager, A., Fehrmann, R.
Pages: 785-789
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Polyhedron
Volume: 30
Issue number: 5
ISSN (Print): 0277-5387
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.02 SJR 0.472 SNIP 0.654
Web of Science (2017): Impact factor 2.067
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.483 SNIP 0.642
Web of Science (2016): Impact factor 1.926
Supported biologically active compounds

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Rodriguez, H., Bica, K., Rogers, R. D., Daly, D. T., Gurau, G.
Publication date: 2011

Publication information
Patent number: WO 2011110662
Date: 15/09/2011
Synergy of boric acid and added salts in the catalytic dehydration of hexoses to 5-hydroxymethylfurfural in water

Boric acid and salts showed a synergistic effect on the dehydration of concentrated aqueous sugar solutions to yield 5-hydroxymethylfurfural.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hansen, T. S., Mielby, J. J., Riisager, A.
Pages: 109-114
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Green Chemistry
Volume: 13
Issue number: 1
ISSN (Print): 1463-9262
Ratings:
- BFI (2019): BFI-level 2
- Web of Science (2019): Indexed yes
- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
- Web of Science (2017): Impact factor 8.586
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
- Web of Science (2014): Impact factor 8.02
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
- Web of Science (2013): Impact factor 6.852
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): CiteScore 6.64 SJR 2.444 SNIP 1.701
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): CiteScore 6.46 SJR 2.32 SNIP 1.641
- Web of Science (2011): Impact factor 6.32
Synthesis of 5-hydroxymethylfurfural and derivatives

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hansen, T. S., Riisager, A.
Publication date: 2011
Peer-reviewed: Yes
Research output: Research - peer-review » Journal article – Annual report year: 2011

Synthesis of 5-(hydroxymethyl)furfural in Ionic Liquids - Paving the Way to Renewable Chemicals
The synthesis of 5-(hydroxymethyl)furfural (HMF) in ionic liquids is a field that has grown rapidly in recent years. Unique dissolving properties for crude biomass in combination with a high selectivity for HMF formation from hexose sugars make ionic liquids attractive reaction media for the production of chemicals from renewable resources. A wide range of new catalytic systems that are unique for the transformation of glucose and fructose to HMF in ionic liquids has been found. However, literature examples of scale-up and process development are still scarce, and future research needs to complement the new chemistry with studies on larger scales in order to find economically and environmentally feasible processes for HMF production in ionic liquids. This Minireview surveys important progress made in catalyst development for the synthesis of HMF in ionic liquids, and proposes future research directions in process technology.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for Process Engineering and Technology, Centre for Catalysis and Sustainable Chemistry
Alkali resistant Fe-zeolite catalysts for SCR of NO with NH3 in flue gases

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Contributors: Putluru, S. S. R., Jensen, A. D., Riisager, A., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Application of Brønsted acid ionic liquids in Pd-catalyzed ethylene alkoxycarbonylation reactions

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., García-Suárez, E. J., Xiong, J., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 2nd Asia Pacific Conference on Ionic Liquids and Green Processes, Dalian, China.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Application of ionic liquid catalysts in the production of biodiesel

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Søndergaard, H., Madsen, A. T., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Application of ionic liquids in fatty acid functionalizations

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Sørensen, M. G., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from Gordon Research Conference on Green Chemistry, Davidson, United States.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Application of ionic Liquids in production of fuel and chemicals from bio-oil

General information
State: Published
Application of Supported Ionic Liquid Phase (SILP) catalysis to Monsanto carbonylation reactions

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hanning, C. W., Fehrmann, R., Riisager, A., Nguyen van Buu, O.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from Green Solvents for Synthesis 2010, Berchtesgaden, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Catalytic and absorption technologies with Supported Ionic Liquid Phase (SILP) materials

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from Pre-symposium Workshop on Commercial Processes and Applications of Ionic Liquids, Dalian, China.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Catalytic conversion of mono- and di-saccharides into ethyl levulinate with Brønsted acid ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Nguyen van Buu, O., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Catalytic flue gas cleaning by solid and liquid ionic media

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2010
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Chemicals from biomass – A new chemical infrastructure

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hansen, T. S., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Designing multifunctional ionic liquids for biomass processing

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kunov-Kruse, A. J., Riisager, A., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes

Event: Abstract from TOKS-XI, Aarhus, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Direct conversion of glucose to 5-(hydroxymethyl)furfural in ionic liquids with lanthanide catalysts
The direct conversion of glucose to 5-(hydroxymethyl)furfural (HMF) in ionic liquids with lanthanide catalysts was examined in search of a possibly more environmentally feasible process not involving chromium. The highest HMF yield was obtained with ytterbium chloride or triflate together with alkylimidazolium chlorides. Notably, a higher reactivity was observed when the hydrophobicity of the imidazolium cation was increased, in contrast to analogous chromium catalyst systems. This indicates a different reaction mechanism for the lanthanides than for the chromium catalyst systems.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T., Sørensen, M. G., Riisager, A.
Pages: 321-325
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Green Chemistry
Volume: 12
Issue number: 2
ISSN (Print): 1463-9262
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.99 SJR 2.496 SNIP 1.847
Web of Science (2017): Impact factor 8.586
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.598 SNIP 2.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.21 SJR 2.452 SNIP 1.884
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 8.05 SJR 2.386 SNIP 1.989
Web of Science (2014): Impact factor 8.02
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 7.44 SJR 2.28 SNIP 1.804
Web of Science (2013): Impact factor 6.852
ISI indexed (2013): ISI indexed yes

Event: Abstract from Green Solvents for Synthesis 2010, Berchtesgaden, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010
Ethylene methoxycarbonylation with palladium-phosphine catalysts in acid-functionalized ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Xiong, J., García-Suárez, E. J., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes

Formation of imines by selective gold-catalysed aerobic oxidative coupling of alcohols and amines under ambient conditions
The formation of imines by aerobic oxidative coupling of mixtures of alcohols and amines was studied using gold nanoparticles supported on titanium dioxide, TiO₂, as a heterogeneous catalyst. The reactions were performed at ambient conditions (room temperature and atmospheric pressure) and occurred with excellent selectivity (above 98%) at moderate conversion under optimized conditions. The effect of catalytic amounts of different bases was studied, along with reaction temperature and time. Utilisation of a selective catalyst system that uses dioxygen as an oxidant and only produces water as by-product represents a new green reaction protocol for imine formation.
Scopus rating (2008): SJR 2.004 SNIP 1.544
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.131 SNIP 1.521
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.554 SNIP 1.414
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.407 SNIP 1.317
Scopus rating (2004): SJR 1.375 SNIP 1.404
Scopus rating (2003): SJR 0.903 SNIP 1.081
Scopus rating (2002): SJR 1.962 SNIP 1.274
Scopus rating (2001): SJR 1.035 SNIP 1.346
Scopus rating (2000): SJR 0.775 SNIP 1.193
Original language: English
DOIs:
10.1039/c0gc00126k
Source: orbit
Source-ID: 265681
Research output: Research - peer-review » Journal article – Annual report year: 2010

Functionalization of fatty acids in ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Sørensen, M. G., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2010

Functionalized ionic liquids: Synthesis, characterization and application

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Søndergaard, H., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from Gordon Research Conference on Green Chemistry, Davidson, United States.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2010

Heteropoly acid promoted Cu and Fe catalysts for the selective catalytic reduction of NO with ammonia

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Putluru, S. S. R., Mossin, S. L., Riisager, A., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 2nd international symposium on air pollution abatement catalysis, Cracow, Poland.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2010

Imine formation by benign oxidative coupling of alcohols and amines using supported gold nanoparticles as catalyst

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kegnæs, S., Mielby, J. J., Mentzel, U. V., Riisager, A.
Publication date: 2010
Ionic liquid gas absorption of NOx, COx and SOx

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Due-Hansen, J., Kegnæs, S., Grétarsdóttir, T., Riisager, A., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Ionic Liquids as Catalysts and Solvents

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Søndergaard, H., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from DTU Chemistry PhD School Symposium 2010, Gentofte, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Ionic Liquids as Catalysts for Biodiesel Synthesis

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Søndergaard, H., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from OChem Autumn School on Green Chemistry, Sønderborg, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Monsanto carbonylation by Supported Ionic Liquid Phase (SILP) catalysis

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hanning, C. W., Fehrmann, R., Riisager, A., Nguyen van Buu, O.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Nanoparticulate metal oxide/anatase catalysts
The present invention concerns a method of preparation of nanoparticulate metal oxide catalysts having a narrow particle size distribution. In particular, the invention concerns preparation of nanoparticulate metal oxide catalyst precursors comprising combustible crystallization seeds upon which the catalyst metal oxide is co-precipitated with the carrier metal oxide, which crystallization seeds are removed by combustion in a final calcining step. The present invention also concerns processes wherein the nanoparticulate metal oxide catalysts of the invention are used, such as SCR (deNOx) reactions of nitrogen oxides with ammonia or urea as reductant, oxidations of alcohols or aldehydes with dioxygen or air to provide aldehydes, ketones or carboxylic acids, and photocatalytic oxidation of volatile organic compounds (VOCs).

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
New catalysts for dehydration of glucose to 5-(hydroxymethyl)furfural in ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T. J. B., Rodriguez, S., Fristrup, P., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

New dual-function catalyst for the dehydration of 5-hydroxy methylfurfural in ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T. J. B., Fristrup, P., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

New ionic liquid catalyst systems for direct dehydration of glucose and its polymers into 5-hydroxymethylfurfural

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Ståhlberg, T. J. B., Riisager, A., Rodriguez, S., Fristrup, P.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from Green Solvents for Synthesis 2010, Berchtesgaden, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

On the importance of the phase distribution and acidity of VOx-ZrO2-SO4-sepiolite catalysts for the NH3-SCR process in relation to biomass fueled power plants

A series of V2O5-ZrO2-SO42- - sepiolite mixtures were extruded, calcined and characterized. NH3-SCR activity was related to the phase distribution of the agglomerant and active VOX-ZrO2-SO42- phase, as well as the acidity of the composite material. Electrophoretic migration results showed that the addition of sepiolite to zirconia had effect on the quantity of zirconia present at the support’s surface, both strongly decreasing the molar fraction of zirconia at the surface, and altering the electrophoretic properties of the mixtures. Addition of extra ammonia sulfate eliminate both effects, and thus facilitate the production of a sepiolite-based confirmed catalyst based on VOx-ZrO2-SO42-, which has been shown to be more resistant to the industrially implemented V2O5-WO3/TO2 catalyst.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Instituto de Catálisis y Petroleoquímica
Contributors: Due-Hansen, J., Rasmussen, S. B., Riisager, A., Ávila, P., Fehrmann, R.
Publication date: 2010
Event information
On the importance of the phase distribution and acidity of VOₓ-ZrO₂-SO₄-sepiolite catalysts for the NH₃-SCR process in relation to biomass fueled power plants

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Due-Hansen, J., Rasmussen, S. B., Riisager, A., Avila, P., Fehrmann, R.
Publication date: 2010
Peer-reviewed: No
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Oxidation of 5-hydroxymethylfurfural with homogeneous Cu(I) catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hansen, T. S., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Oxidation with environmentally benign heterogeneous metal catalysts

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Eyjolfsdottir, E., Kegnæs, S., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Poster session presented at 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Electronic versions:
poster_nsc2010-final.pdf
Source: orbit
Source-ID: 278083
Research output: Research › Poster – Annual report year: 2010

Oxidation with environmentally benign heterogeneous metal catalysts

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Eyjolfsdottir, E., Kegnæs, S., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Process Design for Chemo-enzymatic Synthesis of 2,5-Furandicarboxylic Acid

General information
Process Design for Chemo-enzymatic Synthesis of 2,5-Furandicarboxylic Acid (Best Poster Award)

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Computer Aided Process Engineering Center
Contributors: Fu, W., Jensen, J. S., Boisen, A., Pedersen, S., Riisager, A., Gani, R., Woodley, J.
Publication date: 2010
Peer-reviewed: Yes
Source: orbit
Source-ID: 268762
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Process design for chemo-enzymatic synthesis of 5-hydroxymethylfurfural

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Computer Aided Process Engineering Center
Contributors: Fu, W., Jensen, J. S., Riisager, A., Pedersen, S., Gani, R., Woodley, J.
Publication date: 2010
Event information
Event: BEST 2010
Location: Bologna, Italy
Source: orbit
Source-ID: 267265
Research output: Research › Sound/Visual production (digital) – Annual report year: 2010

Process Design for Chemo-enzymatic Synthesis of 5-Hydroxymethylfurfural

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Sustainable and Green Chemistry, Department of Chemistry, Computer Aided Process Engineering Center, Centre for Catalysis and Sustainable Chemistry
Contributors: Fu, W., Boisen, A., Pedersen, S., Gani, R., Woodley, J., Jensen, J. S., Riisager, A.
Number of pages: 205
Publication date: 2010
Host publication information
Title of host publication: Proceedings of Dansk Kemiingeniørkonference 2010
Source: orbit
Source-ID: 266239
Research output: Research › Article in proceedings – Annual report year: 2010
Renewable building block for plastic industry: Gold-catalyzed oxidation of HMF to FDA in water

Selective amide and imine formation by benign oxidation of alcohols and amines using supported gold nanoparticles as catalyst

Selective flue gas cleaning with ionic liquids
Selective flue gas cleaning with ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kegnæs, S., Due-Hansen, J., Berg, R. W., Riisager, A., Fehrmann, R.
Publication date: 2010
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Selective gas absorption by ionic liquids
Reversible absorption performance for the flue gas components CO₂, NO and SO₂ has been tested for several different ionic liquids (ILs) at different temperatures and flue gas compositions. Furthermore, different porous, high surface area carriers have been applied as supports for the ionic liquids to obtain Supported Ionic Liquid-Phase (SILP) absorber materials. The use of solid SILP absorbers with selected ILs were found to significantly improve the absorption capacity and sorption dynamics at low flue gas concentration, thus making the applicability of ILs viable in technical, continuous flow processes for flue gas cleaning. The results show that CO₂, NO and SO₂ can be reversible and selective absorbed using different ILs and that Supported Ionic Liquid-Phase (SILP) absorbers are promising materials for industrial flue gas cleaning. Absorption/desorption dynamics can be tuned by temperatures, pressures and gas concentrations. © The Electrochemical Society.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark
Contributors: Shunmugavel, S., Kegnæs, S., Due-Hansen, J., Gretasdottir, T., Riisager, A., Fehrmann, R.
Pages: 117-126
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: ECS Transactions
Volume: 33
Issue number: 7
ISSN (Print): 1938-5862
Ratings:
  BFI (2019): BFI-level 1
  Web of Science (2019): Indexed yes
  BFI (2018): BFI-level 1
  BFI (2017): BFI-level 1
  Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
  BFI (2015): BFI-level 1
  Scopus rating (2015): CiteScore 0.36 SJR 0.211 SNIP 0.244
  BFI (2014): BFI-level 1
  Scopus rating (2014): CiteScore 0.36 SJR 0.212 SNIP 0.234
  BFI (2013): BFI-level 1
  Scopus rating (2013): CiteScore 0.27 SJR 0.192 SNIP 0.231
  ISI indexed (2013): ISI indexed no
  BFI (2012): BFI-level 1
  Scopus rating (2012): CiteScore 0.29 SJR 0.241 SNIP 0.26
  ISI indexed (2012): ISI indexed no
  BFI (2011): BFI-level 1
  Scopus rating (2011): CiteScore 0.36 SJR 0.261 SNIP 0.28
Selective gold-catalysed aerobic oxidations under ambient conditions

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kegnæs, S., Mentzel, U. V., Mielby, J. J., Christensen, C. H., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2010

Solubility of CO₂ in functionalized ionic liquid

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Energy Resources Engineering
Contributors: Paul, S., Shunmugavel, S., Riisager, A., Fehrmann, R., Stenby, E. H., Thomsen, K.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from 2010 AIChE Annual Meeting, Salt Lake City, United States.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2010

Supported Ionic Liquid-Phase (SILP) catalysis: New applications with an industrially proven concept

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from EAM Young Researchers’ Day, Germany.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2010

Sustainable plasticizers from bio-oil

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Sørensen, M. G., Riisager, A.
Publication date: 2010
Synthesis and molecular modelling of functionalized ionic liquids for CO₂ capture

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Shunmugavel, S., Paul, S., Thomsen, K., Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from OChem Autumn School on Green Chemistry, Sønderborg, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Towards a sustainable chemical industry based on renewables

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2010
Peer-reviewed: Yes
Event: Abstract from OChem Autumn School, Sønderborg, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Vanadia supported on zeolites for SCR of NO by ammonia
Vanadia supported on zeolites were prepared and characterized by N₂ physisorption, FTIR, XRPD, and NH₃-TPD methods. The influence of the Si/Al ratio on the total surface acidity of the catalysts as well as the optimum V2O5 content were studied and compared with the catalytic activity in the selective catalytic reduction (SCR) of NO with ammonia. The SCR activity was found to correlate directly with the total acidity of the catalysts and showed high poisoning resistivity after doping with potassium oxide (100 μmol/g). The poisoning resistance was due to unique combination of high surface area, acidity and micropore structure of the support. Apparently the support hosted the potassium oxide on the acid sites, thereby protecting the active vanadium species from poisoning. Zeolite based catalysts might therefore prove useful for SCR of NO in alkali-containing flue gases from, e.g. biomass fired power plants.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Putluru, S. S. R., Riisager, A., Fehrmann, R.
Pages: 333-339
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Applied Catalysis B: Environmental
Volume: 97
Issue number: 3-4
ISSN (Print): 0926-3373
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 10.92 SJR 3.152 SNIP 2.359
Web of Science (2017): Impact factor 11.698
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.693 SNIP 2.185
Web of Science (2016): Impact factor 9.446
Original language: English
Keywords: SCR with ammonia, NH3-TPD, Potassium poisoning, Deactivation, Zeolites

DOIs: 10.1016/j.apcatb.2010.04.009
Source: orbit
Source-ID: 270251
Research output: Research - peer-review > Journal article – Annual report year: 2010
X-ray Crystal Structure, Raman Spectroscopy and Ab Initio Density Functional Theory Calculations on 1,1,3,3-Tetramethylguanidinium Bromide

The salt 1,1,3,3-tetramethylguanidinium bromide, \[\text{[(CH}_3\text{)}_2\text{N})_2\text{C}=\text{NH}_2\text{]+Br}^{-}\text{ or [tmgH]Br, was found to melt at 135(5) }^\circ\text{C, forming what may be referred to as a moderate temperature ionic liquid. The chemistry was studied and compared with the corresponding chloride compound.} \]

We present X-ray diffraction and Raman evidence to show that also the bromide salt contains dimeric ion pair “molecules” in the crystalline state and probably also in the liquid state. The structure of \[\text{[tmgH]}\text{Br determined at 120(2) }^\circ\text{K was found to be monoclinic, space group P21/n, with } a = 7.2072(14), b = 13.335(3), c = 9.378(2) \text{ Å, } \beta = 104.31(3)^\circ, Z = 2, \text{ based on 11769 reflections, measured from } \theta = 2.71-28.00^\circ \text{ on a small colorless needle crystal. Raman and IR spectra are presented and assigned. When heated, both the chloride and the bromide salts form vapor phases. The Raman spectra of the vapors are surprisingly alike, showing, for example, a characteristic strong band at 2229 cm}^{-1}. \text{This band was interpreted by some of us to show that the [tmgH]}\text{Cl gas phase should consist of monomeric ion pair “molecules” held together by a single N-H}^{\dagger} \cdot \cdot \cdot \text{Cl}^{-} \text{hydrogen bond, the stretching vibration of which should be causing the band, based on ab initio molecular orbital density functional theory type calculations. It is not likely that both the bromide and chloride should have identical spectra. As explanation, the formation of 1,1-dimethylcyanamidine gas is proposed, by decomposition of [tmgH]}\text{X leaving dimethylammonium halogenide (X = Cl, Br). The Raman spectra of all gas phases were quite identical and fitted the calculated spectrum of dimethylcyanamide. It is concluded that monomeric ion pair “molecules” held together by single N-H}^{\dagger} \cdot \cdot \cdot \text{X}^{-} \text{hydrogen bonds probably do not exist in the vapor phase over the solids at about 200-230 }^\circ\text{C.} \]

General information
State: Published
Organisations: Energy and Materials, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, X-ray Crystallography, Sustainable and Green Chemistry, Fiber Optics, Devices and Non-linear Effects, Department of Photonics Engineering
Contributors: Berg, R. W., Riisager, A., Nguyen van Buu, O., Fehrmann, R., Harris, P., Kristensen, S. B., Brunetti, A. C.
Pages: 13175-13181
Publication date: 2010
Peer-reviewed: Yes

Publication information
Volume: 114
ISSN (Print): 1089-5639
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75 SJR 1.17 SNIP 0.964
Web of Science (2017): Impact factor 2.836
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.252 SNIP 0.958
Web of Science (2016): Impact factor 2.847
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78 SJR 1.148 SNIP 1.074
Web of Science (2015): Impact factor 2.883
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65 SJR 1.159 SNIP 1.069
Web of Science (2014): Impact factor 2.693
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84 SJR 1.205 SNIP 1.109
Web of Science (2013): Impact factor 2.775
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78 SJR 1.513 SNIP 1.127
Web of Science (2012): Impact factor 2.771
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87 SJR 1.422 SNIP 1.131
Web of Science (2011): Impact factor 2.946
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.489 SNIP 1.103
Web of Science (2010): Impact factor 2.732
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.589 SNIP 1.137
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.822 SNIP 1.099
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.951 SNIP 1.139
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.774 SNIP 1.204
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.847 SNIP 1.219
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.711 SNIP 1.233
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.843 SNIP 1.256
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.869 SNIP 1.229
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.826 SNIP 1.202
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.94 SNIP 1.282
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.443 SNIP 1.6
Original language: English
DOIs:
10.1021/jp107152x
Source: orbit
Source-ID: 271724
Research output: Research - peer-review › Journal article – Annual report year: 2010

**Carbonylation in Ionic liquids**

**General information**
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry
Contributors: Riisager, A., Nguyen van Buu, O., Hanning, C., Xiong, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Source: orbit
Source-ID: 257502
Carbonylation reactions using Supported Ionic Liquid Phase (SILP) catalyst technology

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Nguyen van Buu, O., Hanning, C. W., Riisager, A., Haumann, M., Wasserscheid, P., Ha, H. N. T., Le, M. T., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 9th European Congress on Catalysis, Salamanca, Spain.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2009

Catalytic conversion of biomass – A new chemical infrastructure

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Centre for Process Engineering and Technology, Centre for Catalysis and Sustainable Chemistry
Contributors: Hansen, T. S., Woodley, J., Riisager, A.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 9th European Congress on Catalysis, Salamanca, Spain.
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2009

Catalytic conversion of biomass - a new infrastructure

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Sustainable and Green Chemistry, Department of Chemistry
Contributors: Hansen, T., Woodley, J., Riisager, A.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 9th European Congress on Catalysis, Salamanca, Spain.
Source: orbit
Source-ID: 255671
Research output: Research - peer-review » Poster – Annual report year: 2009

Catalytic Dehydration of Glucose In Ionic Liquids

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T. J. B., Sørensen, M. G., Riisager, A.
Publication date: 2009
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2009

Characterization of the surface properties of SILP catalyst

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Ha, H. N. T., Duc, D. T., Dao, T. V., Le, M. T., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Characterization of the surface properties of SILP catalyst

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ha, H. N. T., Duc, D. T., Dao, T. V., Le, M. T., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2009

Conversion of biomass resources into chemicals with integrated catalytic technologies

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, BioChemical Engineering
Contributors: Riisager, A., Søndergaard Hansen, T., Ståhlberg, T., Kegnæs, S., Jensen, J. S., Woodley, J., Boisen, A., Pedersen, S.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from Annual Green Chemistry and Engineering Conference, College Park, MD, USA, .
Source: orbit
Source-ID: 257494
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2009

Conversion of Biomass Resources Into Chemicals with Integrated Catalytic Technologies

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Publication date: 2009

Event information
Event: 13th Annual Green Chemistry and Engineering Conference
Location: College Park, MD, USA, 23-25 June
Source: orbit
Source-ID: 255569
Research output: Research » Sound/Visual production (digital) – Annual report year: 2009

Crystal Structure, Vibrational Spectroscopy and ab Initio Density Functional Theory Calculations on the Ionic Liquid forming 1,1,3,3-Tetramethylguanidinium bis{[trifluoromethyl)sulfonyl]amide
The salt 1,1,3,3-tetramethylguanidinium bis{[trifluoromethyl)sulfonyl]amide, [[[(CH3)2N]2C=NH2]+][N(SO2-CF3)(2)](-) or [tmgH][NTf2], easily forms an ionic liquid with high SO2 absorbing capacity. The crystal structure of the salt was determined at 120(2) K by X-ray diffraction. The structure was found to be monoclinic, space group P2(1)/n with a = 11.349(2), b = 11.631(2), c = 11.887(2) Å, and beta = 90.44(3) degrees. Raman and IR spectra are presented and interpreted. The results are interpreted using ab initio quantum mechanics calculations that also predicted vibrational spectra. The relationship between the transoid (C-2 symmetry) structure of the [NTf2](-) ion and the conformationally sensitive bands is discussed.

General information
State: Published
Organisations: Energy and Materials, Department of Chemistry, Sustainable and Green Chemistry, X-ray Crystallography
Pages: 8878-8886
Publication date: 2009
DeNOx SCR catalysts – mechanism of deactivation and alternative alkali-resistant catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Contributors: Due-Hansen, J., Rasmussen, S. B., Riisager, A., Kustov, A., Fristrup, P., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes

Efficient microwave-assisted synthesis of 5-hydroxymethylfurfural from concentrated aqueous fructose

Studies on the HCl-catalysed microwave-assisted dehydration of highly concentrated aqueous fructose (27 wt %) to 5-hydroxymethylfurfural (HMF) revealed a significant increase in the fructose conversion rate over the conventional heated systems. Water, being the most benign solvent and therefore ideal for green and sustainable chemistry, normally is a poor solvent for the dehydration process resulting in low HMF selectivities and yields. However, reaction at 200 °C with microwave irradiation with a short reaction time of only 1 s resulted in good HMF selectivity of 63% and fructose conversion of 52%, while prolonged irradiation for 60 s (or more) resulted in nearly full fructose conversion (95%) but lower HMF yield (53%). Decreasing the fructose concentration significantly improved the HMF selectivity, but possibly made the production route less attractive from an industrial point of view due to the resultant low throughput.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Søndergaard Hansen, T., Woodley, J., Riisager, A.
Pages: 2568-2572
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Carbohydrate Research
Volume: 344
Issue number: 18
ISSN (Print): 0008-6215
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.02 SJR 0.617 SNIP 0.744
Web of Science (2017): Impact factor 2.074
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.03 SJR 0.659 SNIP 0.796
Web of Science (2016): Impact factor 2.096
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.98 SJR 0.588 SNIP 0.828
Web of Science (2015): Impact factor 1.817
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.01 SJR 0.64 SNIP 0.85
Web of Science (2014): Impact factor 1.929
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.22 SJR 0.64 SNIP 0.852
Web of Science (2013): Impact factor 1.966
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.2 SJR 0.772 SNIP 1.01
Web of Science (2012): Impact factor 2.044
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.43 SJR 0.762 SNIP 1.058
Web of Science (2011): Impact factor 2.332
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.73 SNIP 0.872
Web of Science (2010): Impact factor 1.898
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.888 SNIP 1.024
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.859 SNIP 0.947
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.759 SNIP 0.891
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.643 SNIP 0.903
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.693 SNIP 0.992
Scopus rating (2004): SJR 0.636 SNIP 0.95
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.712 SNIP 0.976
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.77 SNIP 0.948
Web of Science (2002): Indexed yes
Enlarging the surface area of bismuth molybdate containing materials as catalyst of propylene selective oxidation

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Duc, D., Ha, H., Fehrmann, R., Riisager, A., Le, M.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 6th World Congress on Oxidation Catalysis, Lille, France.
Source-ID: 255521
Research output: Research - peer-review › Poster – Annual report year: 2009

Enlarging the surface area of bismuth molybdate containing materials as catalyst of propylene selective oxidation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Duc, D. T., Ha, H. H., Fehrmann, R., Riisager, A., Le, M. T.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 6th World Congress on Oxidation Catalysis, Lille, France.
Source-ID: 257508
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Esterification of free fatty acids in biodiesel production with sulphonated pyrolysed carbohydrate catalysts

The pre-treatment of free fatty acids in oils and fats in biodiesel production is of pivotal importance, and esterification in acidic medium must be done prior to basic transesterification of glycerides. The free fatty acids may be converted over an acidic catalyst of sulphonated pyrolysed carbohydrates. These were prepared by pyrolysis of the carbohydrates in inert atmosphere at 300-450°C in 1-15 h and sulphonation in concentrated or fuming sulphuric acid at 150°C. A monophasic fatty model mixture of lauric acid, tricaprylate and methanol was subsequently treated with the prepared catalysts. Conversion of free fatty acids to methyl esters were monitored by gas chromatography. Sulphonated pyrolysed sugar or starch showed free fatty acid conversions of about 75% in 1 h and about 95% in 3 h.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 9th European Congress on Catalysis, Salamanca, Spain.
Keywords: free fatty acid, biodiesel production, esterification
Source-ID: 257377
Research output: Research - peer-review › Poster – Annual report year: 2009

Esterification of free fatty acids in biodiesel production with sulphonated pyrolysed carbohydrate catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Riisager, A., Fehrmann, R.
Flue Gas Absorption by Tailored Ionic Liquids

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, X-ray Crystallography, Energy and Materials
Contributors: Riisager, A., Harris, P., Berg, R. W., Rogez, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 3rd International Congress on Ionic Liquids, Cairns, Australia.
Source: orbit
Source-ID: 257503
Research output: Research - peer-review › Poster – Annual report year: 2009

Gas-Phase Oxidation of Aqueous Ethanol by Nanoparticle Vanadia/Anatase Catalysts
The gas-phase oxidation of aqueous ethanol with dioxygen has been examined with a new nanoparticle V2O5/TiO2 catalyst. Product selectivity could to a large extent be controlled by small alterations of reaction parameters, allowing production of acetaldehyde at a selectivity higher than 90%, near quantitative conversion at 175-200 A degrees C. Furthermore, a selectivity above 80% for acetic acid could be achieved at low gas hourly space velocity at temperatures as low as 165 A degrees C.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 253-257
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Topics in Catalysis
Volume: 52
Issue number: 3
ISSN (Print): 1022-5528
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.57 SJR 0.965 SNIP 0.753
Web of Science (2017): Impact factor 2.439
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.877
Web of Science (2016): Impact factor 2.486
Gold-Catalyzed Aerobic Oxidation of 5-Hydroxymethylfurfural in Water at Ambient Temperature

The aerobic oxidation of 5-hydroxymethylfurfural, a versatile biomass-derived chemical, is examined in water with a titania-supported gold-nanoparticle catalyst at ambient temperature (30 degrees C). The selectivity of the reaction towards 2,5-furandicarboxylic acid and the intermediate oxidation product 5-hydroxymethyl-2-furancarboxylic acid is found to depend on the amount of added base and the oxygen pressure, suggesting that the reaction proceeds via initial oxidation of the aldehyde moiety followed by oxidation of the hydroxymethyl group of 5-hydroxymethylfurfural. Under optimized reaction conditions, a 71% yield of 2,5-furandicarboxylic acid is obtained at full 5-hydroxymethylfurfural conversion in the presence of excess base.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Gorbanev, Y., Kegnæs, S., Woodley, J., Christensen, C. H., Riisager, A.
Pages: 672-675
Publication date: 2009
Peer-reviewed: Yes
Green aerobic oxidation of HMF

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Gorbanev, Y., Kegnæs, S., Boisen, A., Riisager, A.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from Annual meeting of the Danish Chemical Society, Odense, Denmark.
Research output: Research - peer-review > Conference abstract for conference – Annual report year: 2009

Hydrotreatment of Oils and Fats for Biodiesel

The use of renewable biofuels in the transport sector represents an important step towards a sustainable society. Biodiesel is currently produced by the transesterification of fats and oils with methanol, but another viable method could be reaction of the feedstock with H2 to produce long-chain alkanes. This would allow direct integration of biofuel production in existing refineries and allow use of low-grade feedstock such as abattoir wastes, used fats, greases or even tall oils from the Kraft process. The reaction network from oils and fats in H2 atmosphere includes the direct hydrogenation of the ester or carboxylic acid functionalities with H2 to result in H2O and alkanes (conservation of fatty acid chain length); decarbonylation or decarboxylation of the carboxylic functionality (split-off of CO or CO2, respectively, making the fatty acid chain one C-atom shorter) also yielding alkanes. In all routes propane is formed as a by-product from the glycerol in the fats. The hydrotreatment of a model fat mixture is studied in a stainless steel autoclave between 250 and 375°C, at moderate hydrogen pressures and over catalysts of 5 wt% Pt, Pd or Ni supported on γ-Al2O3. Hydrolysis or hydrogenation of glycerides to free fatty acids is observed to be part of the alkane formation from esters. It was seen that Pt and Pd almost exclusively facilitate the decarbonylation or decarboxylation routes. Ni also facilitated the hydrogenation route, but with a considerably lower overall activity. This may be due to differences in metal particle sizes. While decarbonylation and decarboxylation use least hydrogen during alkane formation itself, the CO and CO2 formed do react with hydrogen to form methane. By GC-analysis of the gas phase after reaction showed that with all tested catalysts, almost all of the CO and CO2 formed yielded CH4. Further investigations of these phenomena are in progress.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Hydrotreatment of Oils and Fats for Biodiesel

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from Annual meeting of the Danish Chemical Society, Odense, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Investigation of Hydrodeoxygenation of Oils and Fats
The use of renewable biofuels in the transport sector represents an important step towards a sustainable society. Biodiesel is currently produced by the transesterification of fats and oils with methanol, but another viable method could be reaction of the feedstock with H2 to produce long-chain alkanes. This would allow direct integration of biofuel production in existing refineries and allow use of feedstock with high amounts of free fatty acids (abattoir wastes, used fats, greases, etc.) [1], or even tall oils from the Kraft process [2]. The reaction network from oils and fats in H2 atmosphere includes the direct hydrogenation of the ester or carboxylic acid functionalities with H2 to result in H2O and alkanes (conservation of fatty acid chain length); decarbonylation or decarboxylation of the carboxylic functionality (split-off of CO or CO2, respectively, making the fatty acid chain one C-atom shorter) also yielding alkanes. In all routes propane is formed as a by-product from the glycerol in the fats. The hydrotreatment of a model fat mixture is studied in a stainless steel autoclave between 250 and 375°C, at moderate hydrogen pressures and over catalysts of 5 wt% Pt, Pd or Ni supported on γ-Al2O3. Hydrolysis or hydrogenation of glycerides to free fatty acids is observed to be part of the alkane formation from esters. It was seen that Pt and Pd almost exclusively facilitate the decarbonylation or decarboxylation routes. Ni also facilitated the hydrogenation route, but with a considerably lower overall activity. This may be due to differences in metal particle sizes. While decarbonylation and decarboxylation use least hydrogen during alkane formation itself, the CO and CO2 formed do react with hydrogen to form methane. By GC-analysis of the gas phase after reaction showed that with all tested catalysts, almost all of the CO and CO2 formed yielded CH4. Further investigations of these phenomena are in progress. 

Ionic liquids as benign solvents for sustainable chemistry

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Riisager, A., Bösmann, A.
Pages: 108-113
Publication date: 2009

Host publication information
Title of host publication: Experiments in Green and Sustainable Chemistry
Volume: 18
Place of publication: Weinheim
Publisher: Wiley-VCH
Editors: Roesky, H. W., Kenneppohl, D.
ISBN (Print): 3-527-32546-8
Source: orbit
Source-ID: 257485
Research output: Research - peer-review › Book chapter – Annual report year: 2009

Ionic Liquids as Reversible Gas Absorbents

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, X-ray Crystallography
Contributors: Riisager, A., Harris, P., Berg, R. W., Rogez, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 35th Conference on Phase Equilibria, Annecy, France.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Ionic liquids as reversible gas absorbers

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, X-ray Crystallography, Energy and Materials
Contributors: Riisager, A., Harris, P., Berg, R. W., Rogez, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 35th Conference on Phase Equilibria, Annecy, France.
Source: orbit
Source-ID: 257490
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Ionic liquids as “solutions” for production of renewable chemicals

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Ståhlberg, T. J. B., Riisager, A.
Publication date: 2009
Kemikalier fra biomasse - når plast gror på træerne

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Contributors: Boisen, A., Hansen, T., Jensen, J., Riisager, A., Woodley, J., Pedersen, S.
Pages: 12-15
Publication date: 2009
Peer-reviewed: Unknown

Publication information
Journal: Dansk Kemi
Volume: 90
Issue number: 4
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
Source: orbit
Source-ID: 255702
Research output: Communication › Journal article – Annual report year: 2009

Model feed for catalytic hydrodeoxygenation of fats for biodiesel production

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from inGAP-NanoCat Summerschool, Trondheim, Norway.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Nano-particle SCR deNOX catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kristensen, S. B., Kunov-Kruse, A. J., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Nano-sized metal oxides as highly active SCR deNOX catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kristensen, S. B., Kunov-Kruse, A. J., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 9th European Congress on Catalysis, Salamanca, Spain.
Palladium-catalyzed methoxycarbonylation of ethylene with acid-functionalized ionic liquids as phase-separable media

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Riisager, A., Xiong, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 9th European Congress on Catalysis, Salamanca, Spain.
Source: orb
Source-ID: 257500

Process integration for the conversion of glucose to 2,5-furandicarboxylic acid
The development of biorefineries means that a key feedstock for many new processes will be sugars in various forms, such as glucose or fructose. From these feedstocks a range of chemicals can be synthesized using heterogeneous catalysis, immobilized enzymes, homogeneous catalysts, soluble enzymes, fermentations or combinations thereof. This presents a particularly interesting process integration challenge since the optimal conditions for each conversion step will be considerably different from each other. Furthermore, compared to oil-based refineries the feedstock represents a relatively high proportion of the final product value and therefore yield and selectivity in these steps are of crucial importance. In this paper using the conversion of glucose to 2,5-furandicarboxylic acid and associated products as an example, alternative routes will be compared with respect to achievable selectivity, and achievable yield.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemical and Biochemical Engineering, Department of Chemistry, Center for BioProcess Engineering, Novozymes AS
Contributors: Boisen, A., Christensen, T., Fu, W., Gorbanev, Y., Hansen, T., Jensen, J., Kegnaes, S., Pedersen, S., Riisager, A., Ståhlberg, T., Woodley, J.
Pages: 1318-1327
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Chemical Engineering Research & Design
Volume: 87
Issue number: 9
ISSN (Print): 0263-8762
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.08 SJR 0.847 SNIP 1.381
Web of Science (2017): Impact factor 2.795
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 0.821 SNIP 1.348
Web of Science (2016): Impact factor 2.538
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.7 SJR 0.852 SNIP 1.434
Web of Science (2015): Impact factor 2.525
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.91 SJR 1.022 SNIP 1.671
Web of Science (2014): Impact factor 2.348
Production of HMF from aqueous fructose – a microwave study

General information
State: Published
Organisations: Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hansen, T., Boisen, A., Woodley, J., Pedersen, S., Riisager, A.
Publication date: 2009

Event information
Raman and DFT Study on N-H+...Cl- Hydrogen Bonding in 1,1,3,3-Tetra-Methylguanidinium Chloride forming an Ion-pair Molecule in the Vapor Phase

The chemistry of 1,1,3,3-tetramethylguanidinium ([TMGH]+) chloride, a low temperature (molten) ionic liquid, is discussed, based on its Raman spectra associated with ab initio molecular orbital DFT-type quantum mechanical calculations (with 6-311+G(d,p) basis sets) on “molecules” in isolated gaseous free states without any assumed symmetry. The calculations on the monomeric [TMGH]+ ion and the dimeric ion pair converged to give geometries near the established crystal structure of the [TMGH]Cl salt. This salt is known to contain dimeric ion pairs of the kind [TMGH][Cl][TMGH](Fig.1). Experimentally obtained Raman scattering spectra of the compound (as the solid, as solutes in ethanolic and aqueous solutions and as a vapor at 225 °C) are presented and assigned, by comparing to the ab initio vibrational analyses (calculated IR and Raman band positions and intensities). It is concluded that dimeric molecular ion pairs with four N-H+...Cl- hydrogen bonds seem to exist also in the solutions, and probably are responsible for the relatively high solubility of the "salt" in ethanol. The "salt" can be easily sublimed at about 200-230 oC. The Raman spectrum of the vapor at 225 °C has a characteristic strong band at 2229 cm⁻¹ that shows that the gas phase consists of monomeric ion pair “molecules” (Fig.2) held together by one N-H+...Cl- hydrogen bond, the stretching band of which is causing the band (Fig.3).

Seed-assisted sol-gel synthesis and characterization of nanoparticular V2O5/anatase

Nanoparticular supported vanadia materials with crystalline anatase support with a narrow size distribution around 12 nm have been synthesized by a new facile sol-gel, co-precipitation method using decomposable ammonium chloride seed crystals. The materials have been characterized by means of X-ray powder diffraction, transmission electron microscopy and nitrogen physisorption. The synthesized high-surface area anatase particles allowed a loading of up to 15 wt.% vanadia without exceeding monolayer coverage of V2O5 in contrast to typical analogous industrial catalysts which only can accommodate 3-5 wt.% vanadia. These materials are promising candidates for improved catalysts for, e.g., oxidation reactions and selective catalytic reduction of NO (X) in flue gases.
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.83 SJR 0.807 SNIP 1.064
Web of Science (2017): Impact factor 2.993
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.49 SJR 0.769 SNIP 1.072
Web of Science (2016): Impact factor 2.599
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.36 SJR 0.792 SNIP 1.059
Web of Science (2015): Impact factor 2.302
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.54 SJR 0.963 SNIP 1.388
Web of Science (2014): Impact factor 2.371
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.36 SJR 0.926 SNIP 1.451
Web of Science (2013): Impact factor 2.305
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.2 SJR 0.988 SNIP 1.383
Web of Science (2012): Impact factor 2.163
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.05 SJR 0.935 SNIP 1.377
Web of Science (2011): Impact factor 2.015
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.957 SNIP 1.091
Web of Science (2010): Impact factor 1.859
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.844 SNIP 0.956
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.68 SNIP 0.773
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.622 SNIP 0.868
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.549 SNIP 0.798
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.561 SNIP 0.879
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.587 SNIP 0.986
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.695 SNIP 1.045
Scopus rating (2002): SJR 0.627 SNIP 0.877
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.734 SNIP 1.015
SILP carbonylation

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hanning, C. W., Nguyen van Buu, O., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from Annual meeting of the Danish Chemical Society, Odense, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Sol-gel method for the preparation of mesoporous materials as supports for the selective oxidation of hydrocarbons

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Le, M. T., Troung, D. D., Nguyen, H. H., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Source: orbit
Source-ID: 257507
Research output: Research - peer-review › Poster – Annual report year: 2009

Sol-gel method for the preparation of mesoporous materials as supports for the selective oxidation of hydrocarbons

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Le, M. T., Truong, D. D., Nguyen, H. H., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Sulfated zirconia as support for alkali-resistant SCR catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Due-Hansen, J., Rasmussen, S. B., Riisager, A., Kustov, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 9th European Congress on Catalysis, Salamanca, Spain.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Supported Ionic Liquid Phase (SILP) Catalyzed Carbonylation Reactions

General information
Supported Ionic Liquid Phase (SILP) Catalyzed Carbonylation Reactions

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Riisager, A., Nguyen van Buu, O., Xiong, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Poster session presented at 3rd International Congress on Ionic Liquids, Cairns, Australia.
Source: orbit
Source-ID: 257504
Research output: Research - peer-review » Poster – Annual report year: 2009

The Effect of Acidic and Redox Properties of V2O5/CeO2-ZrO2 Catalysts in Selective Catalytic Reduction of NO by NH3

V2O5 supported ZrO2 and CeO2–ZrO2 catalysts were prepared and characterized by N2 physisorption, XRPD, TPR, and NH3-TPD methods. The influence of calcination temperature from 400 to 600 °C on crystallinity, acidic and redox properties were studied and compared with the catalytic activity in the selective catalytic reduction (SCR) of NO with ammonia. The surface area of the catalysts decreased gradually with increasing calcination temperature. The SCR activity of V2O5/ZrO2 catalysts was found to be related with the support crystallinity, whereas V2O5/CeO2–ZrO2 catalysts were also dependent on acidic and redox properties of the catalyst. The V2O5/CeO2–ZrO2 catalysts showed high activity and selectivity for reduction of NO with NH3.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Nguyen van Buu, O., Xiong, J., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2009

Publication information
Journal: Catalysis Letters
Volume: 133
Issue number: 3-4
ISSN (Print): 1011-372X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.43 SJR 0.73 SNIP 0.729
Web of Science (2017): Impact factor 2.911
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.755 SNIP 0.786
Web of Science (2016): Impact factor 2.799
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.27 SJR 0.748 SNIP 0.749
Web of Science (2015): Impact factor 2.294
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
The influence of reaction conditions on the humin formation in microwave assisted dehydration of fructose to 5-hydroxymethylfurfural
The synergy effect in the bismuth molybdate based catalysts: The approach from conductivity

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Contributors: Le, M., Van Driessche, I., Hoste, S., Nguyen, H., Truong, D., Riisager, A., Fehrmann, R.
Publication date: 2009
Peer-reviewed: Yes
Event: Abstract from 6th World Congress on Oxidation Catalysis, Lille, France.
Source-ID: 257496
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Udfordringer og strategier ved produktion af biodiesel

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Madsen, A. T., Riisager, A., Fehrmann, R.
Pages: 18-21
Publication date: 2009
Peer-reviewed: Unknown

Publication information
Journal: Dansk Kemi
Volume: 8
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2007): Indexed yes
Web of Science (2004): Indexed yes
Original language: Danish
URLs:
http://www.techmedia.dk/default.asp?Action=Details&Item=552
Source: orbit
Source-ID: 257393
Research output: Communication › Journal article – Annual report year: 2009

Understanding hydrodeoxygenation of oils and fats

Production of diesel fuels from renewable feedstock is increasing. One auspicious route could be by hydrodeoxygenating waste fats and oils to result long-chain alkanes, a process well suited for existing fuel infrastructure. This was studied over metal oxide-supported platinum-group metals in a batch reactor. Oleic acid and tripalmitin in n-tetradecane as a solvent and n-dodecane as internal standard was added to an autoclave and mixed with catalyst and charged with 0-50 bar hydrogen at 250-375°C. This model feed closely resembles waste fats and allows relating the products directly to reactants and reaction routes. Supported Pt and Pd almost exclusively yielded long-chain alkanes via decarboxylation, while complete hydrogenation was suppressed despite high pressures of H2. Deoxygenation without hydrogen was possible as well, although catalysts are prone to faster deactivation. Supported Ni was less active and also consumed more H2 for complete hydrogenation. CH4 was found to be the major component in the gas phase resulting from methanation of H2 and CO or CO2 from decarboxylation. This protocol may be advantageous for studying production of renewable diesel.
Alternative SILP-SCR Catalysts based on Guanidinium Chromates

There is an increasing global concern about human caused emissions of pollutants like sulfur and nitrogen oxides to the atmosphere leading to, e.g. smog and acid rain damaging to the human health and the environment. Selective catalytic reduction (SCR) of NOx with ammonia as reductant is the most efficient method to eliminate NOx from flue gases in stationary sources via the reaction: 4NH3 + 4NO + O2 → 4N2 + 6H2O. The traditionally used heterogeneous SCR catalyst, V2O5-WO3/TiO2, suffers significant deactivation with time due to the presence of relatively large amounts of potassium in the fly ash from bio-fuels. Some of the alkali particles reach the SCR catalyst and deactivate the catalyst both by physical pore blocking as well as by chemically deactivating the oxo vanadium sites. Furthermore, the catalyst operates around 375ºC and thus has to be placed in a certain position in the flue gas duct. There is therefore a demand for alkali-resistant SCR catalysts more flexible regarding temperature of operation and position in the duct. Supported ionic liquid phase (SILP) catalysts with 1,1,3,3-Tetramethylguanidinium (TMGH+) and a chromium oxide anion supported on anatase have exhibited promising low-temperature SCR activity and may possess increased resistance towards potassium poisoning. However, possible drawbacks of applying [TMGH]2Cr2O7 is a reduction in selectivity to N2 in the SCR reaction since the compound is known as an oxidant and may thus contribute to unwanted ammonia oxidation. [TMGH]2Cr2O7 is a solid at ambient conditions, which have allowed X-ray diffraction studies. In this work we present our latest findings regarding the characterization of [TMGH]2Cr2O7 and performance in the SCR reaction.

Bio-Petrochemicals

Catalytic SILP materials

Publication information

Journal: Topics in Organometallic Chemistry
Volume: 23
Continuous, gas-phase hydroformylation of long-chain olefins using supported ionic liquid phase (SILP) catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Nguyen van Buu, O., Nguyen, H., Riisager, A., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Poster session presented at Conference on Molten Salts and Ionic Liquids, Copenhagen, Denmark.
Research output: Research - peer-review > Poster – Annual report year: 2008

Continuous, gas-phase hydroformylation of long-chain olefins using supported ionic liquid phase (SILP) catalysts

General information
Formation of an Ion-Pair Molecule with a Single NH+...Cl- Hydrogen Bond: Raman spectra of 1,1,3,3-Tetramethylguanidinium chloride in the solid state, in solution and in the vapor phase

Some ionic compounds (salts) form liquids when heated to temperatures in the range of 200-300 °C. They may be referred to as moderate temperature ionic liquids. An example of such a compound is the 1,1,3,3- tetramethylguanidinium chloride, [TMGH]Cl, melting at ∼212 °C. The chemistry of this compound containing a dimeric ion-pair "molecule" was investigated in the solid state, in solutions in water and ethanol, and in the vapor phase, based on ab initio molecular orbital density functional theory (DFT)-type calculations with 6-311+G(d,p) basis sets. Calculations on the monomeric [TMGH]+ ion and the dimeric chloride ion-pair salt converged to give geometries near the established crystal structure of [TMGH]Cl. The structures and their binding energies are given as well as calculated vibrational harmonic normal modes (IR and Raman band wavenumbers and intensities). Experimentally obtained Raman scattering spectra are presented and assigned, by comparing to the quantum mechanical calculations. It was discovered that dimeric molecular ion pairs with four N-H+...Cl- hydrogen bonds probably exist in the solutions and are responsible for the relatively high solubility of the "salt" in ethanol. It was discovered that the compound can be easily sublimed by heating to about 200-230 °C. In the Raman spectrum of the vapor at 225 °C, a characteristic strong band at 2229 cm⁻¹ was found and interpreted to show that the gas phase consists of monomeric ion-pair "molecules" held together by a single N-H+...Cl- hydrogen bond, the stretching band of which is causing the band.
Green Aerobic Oxidation of HMF

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering
Contributors: Gorbanev, Y., Kegnæs, S., Christensen, C. H., Boisen, A., Riisager, A.
Publication date: 2008
Highly active SCR deNOx catalysts based on nano-particle vanadia-anatase

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2008
Peer-reviewed: Yes
Event: Poster session presented at Summer School on Green Chemistry, Venice, Italy.
Research output: Research - peer-review › Poster – Annual report year: 2008

Hydroformylation in room temperature ionic liquids (RTILs): Catalyst and process developments

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Haumann, M., Riisager, A.
Pages: 1474-1497
Publication date: 2008
Peer-reviewed: Yes
Publication information
Journal: Chemical Reviews
Volume: 108
Issue number: 4
ISSN (Print): 0009-2665
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 51.08 SJR 23.414 SNIP 11.97
Web of Science (2017): Impact factor 52.613
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 42.79 SJR 19.51 SNIP 10.356
Web of Science (2016): Impact factor 47.928
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 45.92 SJR 18.035 SNIP 11.285
Web of Science (2015): Impact factor 37.369
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 44.56 SJR 18.38 SNIP 11.392
Web of Science (2014): Impact factor 46.568
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 49.12 SJR 22.299 SNIP 12.788
Web of Science (2013): Impact factor 45.661
ISI indexed (2013): ISI indexed yes
I&EC 14-Tuning ionic liquids as high-capacity, reversible gas absorbers for sulphur dioxide

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Energy and Materials
Contributors: Riisager, A., Berg, R. W., Fehrmann, R.
Pages: 14-I&EC PG 1
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Abstract of Papers of the American Chemical Society
Volume: 236
ISSN (Print): 0065-7727
Ratings:
Web of Science (2019): Indexed yes
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed yes
Scopus rating (2014): SJR 0.101 SNIP 0.013
Web of Science (2014): Indexed yes
I&EC 203-Thermomorphic organic liquid-ionic liquid systems: Characterization of phase separation by conductivity and spectroscopy

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Energy and Materials
Contributors: Riisager, A., Berg, R. W., Wasserscheid, P., Fehrmann, R.
Pages: 203-IEC PG 1
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Abstract of Papers of the American Chemical Society
Volume: 236
ISSN (Print): 0065-7727
Ratings:
Web of Science (2019): Indexed yes
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed yes
Scopus rating (2014): SJR 0.101 SNIP 0.013
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.102 SNIP 0
Scopus rating (2009): SJR 0.102 SNIP 0
Ionic Liquids for Reversible Gas Absorption: Absorption Capacity and Structural Characterization

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, X-ray Crystallography
Contributors: Riisager, A., Harris, P., Berg, R. W., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from 214th Meeting of The Electrochemical Society, Honolulu, HI, United States.
Research output: Research - peer-review › Conference abstract in journal – Annual report year: 2008

New insight in the synergy effect of the catalytic system containing bismuth molybdate for selective oxidation of propylene

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Aalborg University
Contributors: Le, M., Van Driessche, I., Hoste, S., Well, W. J. M. V., Nguyen, H., Truong, D., Riisager, A., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Poster session presented at 14th International Congress on Catalysis, Seoul, Korea, Republic of.
Research output: Research - peer-review › Poster – Annual report year: 2008

Reversible gas absorption by ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, X-ray Crystallography
Contributors: Riisager, A., Harris, P., Berg, R. W., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Reversible gas absorption by ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Supported ionic liquid phase (SILP) catalysis and reversible gas absorption

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from Catalysis for Society, Cracow, Poland.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Supported ionic liquid phase (SILP) catalysis in gas-phase hydroformylation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jakuttis, M., Haumann, M., Wasserscheid, P., Riisager, A., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Poster session presented at Jahrestreffen Reaktionstechnik 2008, Würzburg, Germany.
Research output: Research - peer-review › Poster – Annual report year: 2008

Supported ionic liquid phase (SILP) materials for versatile catalytic and gas separation technologies

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Wasserscheid, P., Haumann, M.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from Green Solvents - Progress in Science and Application, Friedrichshafen, Germany.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Supported Ionic Liquid Phase (SILP) Technology: Novel Catalysts and Advanced Materials

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Haumann, M., Wasserscheid, P., Riisager, A., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Supported Ionic Liquid Phase (SILP) Technology – Novel Catalysts and Advanced Materials

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Haumann, M., Wasserscheid, P., Riisager, A., Fehrmann, R.
Pages: 1247
Publication date: 2008
Peer-reviewed: No

Publication information
Journal: Chemie-Ingenieur-Technik
Volume: 80
ISSN (Print): 0009-286X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.51 SJR 0.259 SNIP 0.439
Web of Science (2017): Impact factor 1.1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.83 SJR 0.357 SNIP 0.622
Web of Science (2016): Impact factor 0.877
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.69 SJR 0.343 SNIP 0.585
Web of Science (2015): Impact factor 0.798
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.77 SJR 0.331 SNIP 0.556
Web of Science (2014): Impact factor 0.658
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.62 SJR 0.293 SNIP 0.503
Web of Science (2013): Impact factor 0.661
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.55 SJR 0.34 SNIP 0.531
Web of Science (2012): Impact factor 0.698
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.42 SJR 0.238 SNIP 0.514
Web of Science (2011): Impact factor 0.589
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.211 SNIP 0.342
Web of Science (2010): Impact factor 0.347
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.264 SNIP 0.489
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.2 SNIP 0.283
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.19 SNIP 0.31
Scopus rating (2006): SJR 0.178 SNIP 0.281
Scopus rating (2005): SJR 0.186 SNIP 0.316
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.212 SNIP 0.31
Scopus rating (2003): SJR 0.197 SNIP 0.475
Scopus rating (2002): SJR 0.265 SNIP 0.465
Scopus rating (2001): SJR 0.262 SNIP 0.611
Scopus rating (2000): SJR 0.303 SNIP 0.506
Scopus rating (1999): SJR 0.317 SNIP 0.652
Supported ionic liquid phase (SILP) technology - novel toolbox for homogeneous catalyst immobilization and reaction engineering

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Haumann, M., Wasserscheid, P., Riisager, A.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from Conference on Molten Salts and Ionic Liquids, Copenhagen, Denmark.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Supported Ionic Liquid Phase (SILP) Technology - Novel Toolbox for Homogeneous Catalyst Immobilization and Reaction Engineering

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Haumann, M., Wasserscheid, P., Riisager, A.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from 14th International Congress on Catalysis, Seoul, Korea, Republic of.
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Supported ionic liquids: New versatile catalysts and absorber materials

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Due-Hansen, J., Nguyen van Buu, O., Haumann, M., Wasserscheid, P.
Publication date: 2008
Peer-reviewed: Yes
Event: Poster session presented at 2nd EuCheMS Chemistry Congress, Torino, Italy.
Research output: Research - peer-review › Poster – Annual report year: 2008

Supported liquid catalysts

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Wasserscheid, P.
Pages: 631-644
Publication date: 2008

Host publication information
Title of host publication: Handbook of Heterogeneous Catalysis
Volume: 2
Place of publication: Weinheim
Publisher: Wiley-VCH
Editors: Ertl, G., Knözinger, H., Schüth, F., Weitkamp, J.
Edition: 2
ISBN (Print): 3527312412, 978-3527312412
Source: orbit
Source-ID: 233333
Research output: Research - peer-review › Book chapter – Annual report year: 2008
Thermomorphic organic liquid-ionic liquid systems: Characterization of phase separation by conductivity and spectroscopy

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Berg, R. W., Wasserscheid, P., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from Ionic Liquids: From Knowledge to Application, Philadelphia, (PA), United States.
Research output: Research › peer-review › Conference abstract for conference – Annual report year: 2008

Tuning ionic liquids as high-capacity, reversible gas absorbers for sulphur dioxide

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Berg, R. W., Fehrmann, R.
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from Ionic Liquids: From Knowledge to Application, Philadelphia, (PA), United States.
Research output: Research › peer-review › Conference abstract for conference – Annual report year: 2008

Tuning ionic liquids for high gas solubility and reversible gas sorption
New 1,1,3,3-tetramethylguanidinium-based ionic liquids have been synthesized and their ability to reversibly absorb gaseous sulfur dioxide and ammonia investigated. It was found that up to 2 moles of gas at 1 bar could be absorbed per mole of ionic liquid at room temperature and almost completely desorbed by heating or lowering of the pressure. No change in absorbing capacity of the ionic liquids was observed after several cycles. The absorption of SO₂ in the ionic liquids is an exothermic process and standard enthalpy of solution was found to be in the range −21 to −37 kJ mol⁻¹, indicating a moderate association between gas and liquid, which also could be confirmed by Raman and UV–vis spectroscopy on the gas-saturated (1 bar) ionic liquids. Knowledge of gas solubilities and the reversible gas absorption capacity of ionic liquids is believed to have importance for their possible application as reaction media for, e.g. catalytic processes involving gaseous reactants, and as absorbents in gas separation processes.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Energy and Materials
Contributors: Huang, J., Riisager, A., Berg, R. W., Fehrmann, R.
Pages: 170-176
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Journal of Molecular Catalysis A: Chemical
Volume: 279
Issue number: 2
ISSN (Print): 1381-1169
Ratings:
BFI (2019): BFI-level 1
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Impact factor 4.397
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.96 SJR 1.006 SNIP 1.095
Web of Science (2016): Impact factor 4.211
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.93 SJR 1.052 SNIP 1.262
Web of Science (2015): Impact factor 3.958
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.93 SJR 1.092 SNIP 1.431
V$_2$O$_5$-based NH$_3$-SCR Catalysts Doped with Potassium

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Publication date: 2008
Alternative flue gas cleaning by catalysis, electrocatalysis and selective gas absorption

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 210002
Research output: Research › Conference abstract for conference – Annual report year: 2007

Continuous gas-phase hydroformylation of 1-butene using supported ionic liquid phase (SILP) catalysts

The concept of supported ionic liquid phase (SILP) catalysis has been extended to 1-butene hydroformylation. A rhodium-sulfoxantphos complex was dissolved in [BMIM][n-C8H17OSO3] and this solution was highly dispersed on silica. Continuous gas-phase experiments in a fixed-bed reactor revealed these SILP catalysts to be highly active, selective and long-term stable. Kinetic data have been acquired by variation of temperature, pressure, syngas composition, substrate and catalyst concentration. A linear dependency in rhodium concentration could be established over a large concentration range giving another excellent hint for truly homogeneous catalysis in the SILP system. Compared to former studies using propene, the SILP system showed significantly higher activity and selectivity with 1-butene as feedstock. These findings could be elucidated by solubility measurements using a magnetic microbalance.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Haumann, M., Dentler, K., Joni, J., Riisager, A., Wasserscheid, P.
Pages: 425-431
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Advanced Synthesis and Catalysis
Volume: 349
Issue number: 3
ISSN (Print): 1615-4150
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 5.01 SJR 2.079 SNIP 0.935
Web of Science (2017): Impact factor 5.123
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.36 SJR 2.416 SNIP 0.948
Web of Science (2016): Impact factor 5.646
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 6.07 SJR 2.59 SNIP 1.102
Continuous SILP catalysis – An efficient and solvent-free concept for homogeneously catalyzed reactions.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Haumann, M., Wasserscheid, P., Fehrmann, R., Riisager, A.
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 210001
Research output: Research › Conference abstract for conference – Annual report year: 2007
Fixed-bed reactor cascades using homogeneous catalysts immobilized via Supported Ionic Liquid Phase (SILP) technology

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at 13th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Berkeley, United States.
Research output: Research - peer-review > Poster – Annual report year: 2007

Flue Gas Cleaning With Alternative Processes and Reaction Media
Alternative methods to the traditional industrial NOX and SOX flue gas cleaning processes working at lower temperatures and/or leading to useful products are desired. In this work we present our latest results regarding the use of molten ionic media in electrocatalytic membrane separation, ionic liquid reversible absorption and supported ionic liquid deNOX catalysis. Further development of the methods will hopefully make them suitable for installation in different positions in the flue gas duct as compared to the industrial methods available today.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 49-59
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: E C S Transactions
Volume: 3
Issue number: 35
ISSN (Print): 1938-5862
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.36 SJR 0.211 SNIP 0.244
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.36 SJR 0.212 SNIP 0.234
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.27 SJR 0.192 SNIP 0.231
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.29 SJR 0.241 SNIP 0.26
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.36 SJR 0.261 SNIP 0.28
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Formation of Acetic Acid and Ethyl Acetate by Gold Catalysed Oxidation of Ethanol

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Hansen, J. R., Egeblad, K., Riisager, A., Christiansen, S., Dahl Thomsen, M., Christensen, C. H.
Publication date: 2007
Peer-reviewed: Yes
Research output: Research - peer-review › Poster – Annual report year: 2007

Gold Catalysed Aqueous-Phase Oxidation of Bioethanol

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Hansen, J. R., Egeblad, K., Riisager, A., Christensen, C. H.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at Eurocombicat 2007, Bari, Italy.
Research output: Research - peer-review › Poster – Annual report year: 2007

Gold Catalyzed Aerobic Oxidation of Ethanol: A Sustainable Path to Commodity Chemicals

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Hansen, J. R., Egeblad, K., Christiansen, S., Dahl Thomsen, M., Riisager, A., Christensen, C. H.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at 8th European Congress on Catalysis, Turku, Finland.
Research output: Research - peer-review › Poster – Annual report year: 2007

Ioniske væsker: Fremtidens designersolventer

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Low temperature selective catalytic reduction (SCR) of NO with NH3 over alternative metal oxide-based catalysts

General information
State: Published
Organisations: Department of Chemistry
Contributors: Hamma-Cugny, H., Huang, J., Riisager, A., Rasmussen, S. B., Fehrmann, R.
Publication date: 2007
Peer-reviewed: Yes
Event: Abstract from 8th European Congress on Catalysis, Turku, Finland.
Source: orbit
Source-ID: 210458
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2007

Low temperature selective catalytic reduction (SCR) of NO with NH3 over alternative metal oxide-based catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hamma-Cugny, H., Huang, J., Riisager, A., Rasmussen, S. B., Fehrmann, R.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at 8th European Congress on Catalysis, Turku, Finland.
Research output: Research - peer-review › Poster – Annual report year: 2007

Low temperature selective catalytic reduction (SCR) of NO with NH3 over alternative metal oxide-based catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Hamma-Cugny, H., Riisager, A., Fehrmann, R., Rasmussen, S. B., Huang, J.
Publication date: 2007
Peer-reviewed: Yes
Research output: Research - peer-review › Poster – Annual report year: 2007

Nano-particle Vanadia-Anatase SCR deNOX Catalysts

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Kristensen, S. B., Kruse, A., Riisager, A., Rasmussen, S. B., Hamma-Cugny, H., Fehrmann, R.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at 20th North American Catalysis Society Meeting (NACS), Houston, TX, United States.
Research output: Research - peer-review › Poster – Annual report year: 2007
New Process Opportunities in Catalysis and Separation Technology with Supported Ionic Liquid Phase (SILP) Systems

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Fehrmann, R., Riisager, A., Hamma-Cugny, H., Haumann, M., Wasserscheid, P.
Publication date: 2007
Peer-reviewed: Yes
Research output: Research - peer-review › Poster – Annual report year: 2007

Novel metal oxide catalysts for low temperature selective catalytic reduction

General information
State: Published
Organisations: Department of Chemistry
Contributors: Hamma-Cugny, H., Riisager, A., Fehrmann, R., Rasmussen, S. B., Huang, J.
Publication date: 2007
Peer-reviewed: Yes
Event: Abstract from European Congress of Chemical Engineering - 6, Copenhagen, Denmark.
Source: orbit
Source-ID: 210456
Research output: Research - peer-review › Conference abstract for conference – Annual report year: 2007

SILP Catalysis – An innovative concept for benign continuous, solvent-free processes using ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2007
Peer-reviewed: No
Event: Abstract from European Congress of Chemical Engineering - 6, Copenhagen, Denmark.
Source: orbit
Source-ID: 210004
Research output: Research › Conference abstract for conference – Annual report year: 2007

Supported ionic liquid phase catalysts

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrmann, R.
Pages: 527-558
Publication date: 2007

Host publication information
Title of host publication: Ionic Liquids in Synthesis : Completely revised and enlarged Edition
Volume: Chapter 5.6
Place of publication: Weinheim
Supported Ionic Liquid Phase Catalysts for \( \text{NO}_x \) and \( \text{SO}_2 \) Removal

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Due-Hansen, J., Riisager, A., Hamma-Cugny, H., Fehrmann, R.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at Summer School, Sandbjerg, Denmark.
Research output: Research - peer-review \( \rightarrow \) Poster – Annual report year: 2007

Supported Ionic Liquid Phase (SILP) catalysis in gas-phase hydroformylation

General information
State: Published
Organisations: Department of Chemistry
Contributors: Jakuttis, M., Haumann, M., Wasserscheid, P., Riisager, A., Fehrmann, R.
Publication date: 2007
Peer-reviewed: Yes
Event: Abstract from 8th European Congress on Catalysis, Turku, Finland.
Source: orbit
Source-ID: 210457
Research output: Research - peer-review \( \rightarrow \) Conference abstract for conference – Annual report year: 2007

Supported Ionic Liquid Phase (SILP) catalysis in gas-phase hydroformylation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jakuttis, M., Haumann, M., Wasserscheid, P., Riisager, A., Fehrmann, R.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at 8th European Congress on Catalysis, Turku, Finland.
Research output: Research - peer-review \( \rightarrow \) Poster – Annual report year: 2007

Supported ionic liquid phase (SILP) systems - novel fixed bed reactor concepts for homogeneous catalysis

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Jakuttis, M., Joni, J., Wasserscheid, P.
Pages: 139-143
Publication date: 2007

Host publication information
Title of host publication: Proceedings of the 15th Conference of the Petrochemistry Division of DGMK: Opportunities and Challenges at the Interface between Petrochemistry and Refinery
Source: orbit
Source-ID: 209999
Research output: Research - peer-review \( \rightarrow \) Article in proceedings – Annual report year: 2007

Supported Ionic Liquid Phase (SILP) Technology: A Platform Technology for Catalyst Immobilization

General information
Supported ionic liquid phase (SILP) technology for new process designs

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2007
Peer-reviewed: Yes
Event: Poster session presented at 13th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Berkeley, United States.
Research output: Research - peer-review » Poster – Annual report year: 2007

Supported Ionic Liquid Phase (SILP) Technology – From Immobilized Catalysts to Advanced Materials

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrmann, R.
Publication date: 2007
Peer-reviewed: No
Source: orbit
Source-ID: 210000
Research output: Research » Conference abstract for conference – Annual report year: 2007

The SILP (Supported Ionic Liquid Phase) Concept - Recent Developments within Catalysis and Reversible Gas Absorption

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Energy and Materials
Contributors: Riisager, A., Hamma-Cugny, H., Berg, R. W., Fehrmann, R.
Publication date: 2007
Peer-reviewed: No
Event: Abstract from 8th European Congress on Catalysis, Turku, Finland.
Source: orbit
Source-ID: 210003
Research output: Research » Conference abstract for conference – Annual report year: 2007

Bæredygtig Eddikesyre

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Hansen, J. R., Egeblad, K., Kegnæs, S., Riisager, A., Christensen, C. H.
Publication date: 2006
Peer-reviewed: Yes
Event: Poster session presented at Kemisk Forenings Årsmøde, Odense, Denmark.
Research output: Research - peer-review » Poster – Annual report year: 2006
Catalytic SILP materials for selective, continuous gas-phase hydroformylation of 1-olefins

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Haumann, M., Wasserscheid, P., Fehrmann, R., Riisager, A.
Publication date: 2006
Peer-reviewed: No
Event: Poster session presented at 15th International Symposium on Homogeneous Catalysis, Sun City, South Africa.
Source: orbit
Source-ID: 194544
Research output: Research › Poster – Annual report year: 2006

Catalytic SILP materials for the continuous gas-phase hydroformylation of 1-olefins

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2006
Peer-reviewed: No
Event: Poster session presented at Green Solvents for Processes, Lake Constance, Germany.
Source: orbit
Source-ID: 194547
Research output: Research › Poster – Annual report year: 2006

Continuous, gas-phase oxidation of bio-ethanol with air using gold catalysts: A green and sustainable process to make acetic acid

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2006
Peer-reviewed: No
Event: Poster session presented at 1st International IUPAC Conference on Green-Sustainable Chemistry, Dresden, Germany.
Source: orbit
Source-ID: 194545
Research output: Research › Poster – Annual report year: 2006

DeNOX and deSOX of flue gases by catalysis, electrocatalysis and selective gas absorption using ionic media

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Laboratoire TECSEN, Georgia Institute of Technology, Friedrich-Alexander University Erlangen-Nürnberg
Publication date: 2006
Peer-reviewed: No
Source: orbit
Source-ID: 194541
Research output: Research › Conference abstract for conference – Annual report year: 2006

Ethanol as a renewable feedstock for commodity chemicals: Acetic acid as an example

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Rass-Hansen, J., Riisager, A., Egeblad, K., Christensen, C. H.
First application of supported ionic liquid phase (SILP) catalysis for continuous methanol carbonylation

A solid, silica-supported ionic liquid phase (SILP) rhodium iodide Monsanto-type catalyst system, [BMIM][Rh(CO)(2)I-2]-[BMIM]I-SiO2, exhibits excellent activity and selectivity towards acetyl products in fixed-bed, continuous gas-phase methanol carbonylation.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Jørgensen, B., Wasserscheid, P.
Pages: 994-996
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Chemical Communications
Issue number: 9
ISSN (Print): 1359-7345
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127
Web of Science (2017): Impact factor 6.29
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.06 SJR 2.538 SNIP 1.16
Web of Science (2016): Impact factor 6.319
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.7 SJR 2.601 SNIP 1.295
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.83 SJR 2.692 SNIP 1.436
Web of Science (2014): Impact factor 6.834
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.73 SJR 2.752 SNIP 1.372
Web of Science (2013): Impact factor 6.718
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.21 SJR 3.118 SNIP 1.35
Web of Science (2012): Impact factor 6.378
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Flue Gas Cleaning With Alternative Processes and Reaction Media

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry
Contributors: Fehrmann, R., Hamma-Cugny, H., Riisager, A., Huang, J., Rogez, J., Rasmussen, S. B.
Pages: Abstract 1994
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
Fehrmann.pdf
Source: orbit
Source-ID: 264236
Research output: Research - peer-review › Conference abstract in journal – Annual report year: 2006
Formation of Acetic Acid by Aqueous-Phase Oxidation of Ethanol with Air in the Presence of a Heterogeneous Gold Catalyst

Die selektive Oxidation von Ethanol zu Essigsäure gelingt in wässriger Lösung mit dem Oxidans Luft an einem Gold-Heterogenkatalysator (siehe Bild). Bei 423 K und einem O2-Druck von 0.6 MPa verläuft diese Reaktion glatt in saurer wässriger Lösung in Ausbeuten um 90%. CO2 ist das einzige Nebenprodukt, das in nennenswerten Mengen entsteht.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 4764–4767
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Angewandte Chemie
Volume: 118
Issue number: 28
ISSN (Print): 0044-8249
Ratings:
BFI (2019): BFI-level 1
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
BFI (2009): BFI-level 1
BFI (2008): BFI-level 1
Web of Science (2008): Indexed yes
Original language: English
Keywords: Bioethanol, Essigsäure, Gold, Heterogene Katalyse, Oxidationen
DOIs:
10.1002/ange.200601180
Research output: Research - peer-review › Journal article – Annual report year: 2006

Gold Catalysed Aqueous-Phase Oxidation of Ethanol by Air

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Hansen, J. R., Egeblad, K., Kegnæs, S., Riisager, A., Christensen, C. H.
Publication date: 2006
Peer-reviewed: Yes
Event: Poster session presented at Surface reactivity and Nanocatalysis Summer School, Ebeltoft, Denmark.
Research output: Research - peer-review › Poster – Annual report year: 2006
Ionic liquids: Benign reaction media for homogeneous catalysis

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from 2006 Annual meeting of the Danish Chemical Society, Odense, Denmark.
Source: orbit
Source-ID: 194550
Research output: Research › Conference abstract for conference – Annual report year: 2006

Ionic Liquids: Benign Solvents for Supported Liquid Catalyst Systems

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2006
Peer-reviewed: No
Source: orbit
Source-ID: 194538
Research output: Research › Conference abstract for conference – Annual report year: 2006

Nano-sized metal/metal oxides in supported ionic liquid catalysis

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, Friedrich-Alexander University Erlangen-Nürnberg
Publication date: 2006
Peer-reviewed: No
Event: Poster session presented at Green Solvents for Processes, Lake Constance, Germany.
Source: orbit
Source-ID: 194546
Research output: Research › Poster – Annual report year: 2006

Reversible physical absorption of SO2 by ionic liquids
Ionic liquids can reversibly absorb large amounts of molecular SO2 gas under ambient conditions with the gas captured in a restricted configuration, possibly allowing SO2 to probe the internal cavity structures in ionic liquids besides being useful for SO2 removal in pollution control.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Huang, J., Riisager, A., Fehrmann, R., Wasserscheid, P.
Pages: 4027-4029
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Chemical Communications
Issue number: 38
ISSN (Print): 1359-7345
Ratings:
BFI (2019): BFI-level 2
SILP catalysis in gas-phase hydroformylation and carbonylation

General information
State: Published
Organisations: Department of Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Pages: 57-63
Publication date: 2006

Host publication information
Title of host publication: Proceeding of the 14th Conference of Petrochemistry Division of DGMK : Synthesis Gas Chemistry
Source: orbit
Source-ID: 194527
Research output: Research › Article in proceedings – Annual report year: 2006

SILP catalysis in gas-phase hydroformylation and carbonylation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Pages: 695-706
Publication date: 2006
Peer-reviewed: Yes
Event: Abstract from 14th Conference of the Petrochemistry Division of DGMK, Dresden, Germany.
Research output: Research › Conference abstract for conference – Annual report year: 2006

Supported Ionic Liquid Phase (SILP) catalysis: An innovative concept for homogeneous catalysis in continuous fixed-bed reactors

Applications of ionic liquids to replace conventional solvents in homogeneous transition-metal catalysis have increased significantly during the last decade. Biphasic ionic liquid/organic liquid systems offer advantages with regard to product separation, catalyst stability, and recycling but utilise in the case of fast chemical reactions only a small amount of expensive ionic liquid and catalyst. The novel Supported Ionic Liquid Phase (SILP) catalysis concept overcomes these drawbacks and allows the use of fixed-bed reactors for continuous reactions. In this Microreview the SILP catalysis concept is surveyed by presenting results for the continuous gas-phase hydroformylation of propene, as a reaction example. (c) Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, Germany, 2006.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Pages: 695-706
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: European Journal of Inorganic Chemistry
Supported ionic liquid phase (SILP) catalysis: A new concept for continuous, fixed-bed methanol carbonylation

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Jørgensen, B., Haumann, M., Wasserscheid, P., Fehrmann, R.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from 12th Nordic Symposium on Catalysis, Trondheim, Norway.
Source: orbit
Source-ID: 194497
Research output: Research › Review – Annual report year: 2006

Supported Ionic Liquid Phase (SILP) catalysis: An innovative concept for homogeneous catalysis in continuous fixed bed reactors.

**General information**
State: Published
Organisations: Department of Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from 39th Jahrestreffen Deutscher Katalytiker, .
Source: orbit
Source-ID: 194532
Research output: Research › Conference abstract for conference – Annual report year: 2006

Supported ionic liquid phase (SILP) catalysis - A promising new industrial process design?

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Jørgensen, B., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2006
Peer-reviewed: No
Event: Abstract from 231th American Chemical Society National Meeting, Atlanta, United States.
Source: orbit
Source-ID: 194534
Research output: Research › Conference abstract for conference – Annual report year: 2006

Supported ionic liquid phase (SILP) catalysis - A promising new industrial process design?

**General information**
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R.
Publication date: 2006
Peer-reviewed: No
Supported Ionic Liquid Phase (SILP) catalysis – a versatile concept for continuous, homogeneous solvent-free processes

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2006
Peer-reviewed: No
Event: Poster session presented at 15th International Symposium on Homogeneous Catalysis, Sun City, South Africa.
Source: orbit
Source-ID: 194543
Research output: Research - poster – Annual report year: 2006

Supported ionic liquid-phase (SILP) catalysts in continuous flow processes

General information
State: Published
Organisations: Department of Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Flicker, S., Haumann, M., Wasserscheid, P., Fehrmann, R.
Pages: 630-638
Publication date: 2006

Host publication information
Title of host publication: Proceedings of the 14th International Symposium on Molten Salts : 206th Meeting of the Electrochemical Society
Source: orbit
Source-ID: 194530
Research output: Research - article in proceedings – Annual report year: 2006

Supported ionic liquid: versatile reaction and separation media
The latest developments in supported ionic liquid phase (SILP) systems for catalysis and separation technology are surveyed. The SILP concept combines the advantages of homogeneous catalysis with heterogeneous process technology, and a variety of reactions have been studied where supported ionic liquid catalysts proved to be more active.
and selective than common systems. In separation applications the use of supported ionic liquids can facilitate selective transport of substrates across membranes.

**General information**

State: Published  
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Friedrich-Alexander University Erlangen-Nürnberg  
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.  
Pages: 91-102  
Publication date: 2006  
Peer-reviewed: Yes

**Publication information**

Journal: Topics in Catalysis  
Volume: 40  
Issue number: 1-4  
ISSN (Print): 1022-5528  
Ratings:  
BFI (2019): BFI-level 1  
Web of Science (2019): Indexed yes  
BFI (2018): BFI-level 1  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 2.57 SJR 0.965 SNIP 0.753  
Web of Science (2017): Impact factor 2.439  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.55 SJR 0.975 SNIP 0.877  
Web of Science (2016): Impact factor 2.486  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): CiteScore 2.41 SJR 0.926 SNIP 0.777  
Web of Science (2015): Impact factor 2.355  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): CiteScore 2.29 SJR 0.987 SNIP 0.845  
Web of Science (2014): Impact factor 2.365  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): CiteScore 2.67 SJR 1.119 SNIP 0.827  
Web of Science (2013): Impact factor 2.22  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): CiteScore 2.49 SJR 1.196 SNIP 0.848  
Web of Science (2012): Impact factor 2.608  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): CiteScore 2.89 SJR 1.338 SNIP 0.965  
Web of Science (2011): Impact factor 2.624  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.506 SNIP 0.919  
Web of Science (2010): Impact factor 2.359  
Web of Science (2010): Indexed yes
Sustainable Acetic acid

General information
State: Published
Organisations: Department of Chemistry, Technical University of Denmark
Publication date: 2006
Peer-reviewed: No
Event: Poster session presented at 2006 Annual meeting of the Danish Chemical Society, Odense, Denmark.
Source: orbit
Source-ID: 194504
Research output: Research - peer-review › Journal article – Annual report year: 2006

Sustainable and Green Aqueous-phase Oxidation of Bioethanol to Acetic Acid Using Gold Catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2006
Peer-reviewed: No
Event: Abstract from 1st International IUPAC Conference on Green-Sustainable Chemistry, Dresden, Germany.
Source: orbit
Source-ID: 194551
Research output: Research › Conference abstract for conference – Annual report year: 2006

Sustainable, gas-phase methanol carbonylation with supported ionic liquid phase (SILP) catalysis

General information
State: Published
A truly homogeneous catalyst in heterogeneous form - the supported ionic liquid phase (SILP) catalyst concept for continuous, gas-phase propene hydroformylation

General information
State: Published
Organisations: Department of Chemistry, Friedrich-Alexander University Erlangen-Nürnberg
Contributors: Riisager, A., Flicker, S., Fehrmann, R., Hauman, M., Gorle, B. S., Wasserscheid, P.
Pages: 1210-1210
Publication date: Aug 2005
Peer-reviewed: No

Publication information
Journal: Chemie-Ingenieur-Technik
Volume: 77
Issue number: 8
ISSN (Print): 0009-286X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.51 SJR 0.259 SNIP 0.439
Web of Science (2017): Impact factor 1.1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.83 SJR 0.357 SNIP 0.622
Web of Science (2016): Impact factor 0.877
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.69 SJR 0.343 SNIP 0.585
Web of Science (2015): Impact factor 0.798
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.77 SJR 0.331 SNIP 0.556
Web of Science (2014): Impact factor 0.658
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.62 SJR 0.293 SNIP 0.503
Web of Science (2013): Impact factor 0.661
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.55 SJR 0.34 SNIP 0.531
Web of Science (2012): Impact factor 0.698
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.42 SJR 0.238 SNIP 0.514
Web of Science (2011): Impact factor 0.589
ISI indexed (2011): ISI indexed yes
A truly homogeneous catalyst in heterogeneous form - The supported ionic liquid phase (SILP) catalyst concept for continuous, gas-phase propene hydroformylation

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Gorle, B. S., Wasserscheid, P., Haumann, M.
Publication date: 2005
Peer-reviewed: No
Event: Abstract from 12th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, Florence, Italy, .
Source: orbit
Source-ID: 188125
Research output: Research › Conference abstract for conference – Annual report year: 2005

Catalysis in ionic media

General information
State: Published
Organisations: Department of Chemistry
Contributors: Fehrmann, R., Riisager, A., Rasmussen, S. B.
Number of pages: 5
Publication date: 2005

Host publication information
Title of host publication: Proc., 7th Int. Symp. Molten Salts Chemistry and Technology
Source: orbit
Source-ID: 188011
Research output: Research - peer-review › Article in proceedings – Annual report year: 2005

Catalysis in ionic media

General information
First very stable and highly regioselective supported ionic liquid-phase (SILP) catalysis: Continuous-flow fixed-bed hydrofomylation of propene

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Riisager, A., Rasmussen, S. B.
Publication date: 2005
Peer-reviewed: Yes
Event: Abstract from 7th International Symposium Molten Salts Chemistry and Technology, Toulouse, France.
Research output: Research - peer-review > Conference abstract for conference – Annual report year: 2005

Publication Information
Journal: Angewandte Chemie International edition
Volume: 44
Issue number: 5
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Impact factor 12.102
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.146
Web of Science (2016): Impact factor 11.994
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.13 SJR 5.888 SNIP 2.225
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 10.84 SJR 5.811 SNIP 2.307
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.7 SJR 5.702 SNIP 2.198
Web of Science (2013): Impact factor 11.336
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.55 SJR 6.407 SNIP 2.329
Web of Science (2012): Impact factor 13.734
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 10.75 SJR 6.063 SNIP 2.361
Web of Science (2011): Impact factor 13.455
New Applications of Supported Ionic Liquid-Phase (SILP) Catalysts in Continuous flow Processes.

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Wasserscheid, P.
Publication date: 2005
Peer-reviewed: No
Source: orbit
Source-ID: 188007
Research output: Research – Conference abstract for conference – Annual report year: 2005

Stability and kinetic studies of supported ionic liquid phase catalysts for hydroformylation of propene
Supported ionic liquid phase (SILP) catalysts have been studied with regard to their long-term stability in the continuous gas-phase hydroformylation of propene. Kinetic data have been acquired by variation of temperature, pressure, syngas composition, substrate concentration, and residence time. The activation energy was determined to be 63.3 ± 2.1 kJ mol⁻¹, which is in good agreement with known results from biphasic hydroformylation. The results from the kinetic studies confirmed previously published results on the homogeneous nature of the heterogenised Rh-SILP catalyst. Long-term stability exceeded 200 h time on stream with no loss in selectivity. A small decrease in activity could be compensated by a vacuum procedure regaining the initial activity.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Haumann, M., Gorle, B. S., Wasserscheid, P.
Supported ionic liquid-phase (SILP) catalysis: Heterogenization of homogeneous rhodium phosphine catalysts.
The concept of supported ionic liquid-phase (SILP) catalysis has been demonstrated for gas- and liquid-phase continuous
fixed-bed reactions using rhodium phosphine catalyzed hydroformylation of propene and 1-octene as examples. The
nature of the support had important influence on both the catalytic performance, i.e. activity and selectivity, as well as
stability of the SILP catalysts. Noticeably, a high catalyst ligand content together with presence of ionic liquid solvent are
prerequisites for obtaining selective rhodium phosphine SILP catalysts systems.

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Wasserscheid, P., van Hal, R.
Pages: 334-349
Publication date: 2005

Host publication information
Title of host publication: Ionic Liquids IIIB: : Fundamentals, Progress, Challenges, and Oppertunities -Transformations and
Processes
Volume: 902
ISBN (Print): 9780841238947
ISBN (Electronic): 9780841220201
(ACS Symposium Series).
DOIs:
10.1021/bk-2005-0902.ch023
Source: orbit
Source-ID: 199304
Research output: Research › Book chapter – Annual report year: 2005

Supported ionic liquid-phase (SILP) catalysis – Heterogenization of homogeneous rhodium phosphine catalysts

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Wasserscheid, P., van Hal, R.
Pages: 334-349
Publication date: 2005
Host publication information
Title of host publication: Ionic Liquids III: Fundamentals, Progress, Challenges, and Opportunities - Transformations and Processes
Volume: Chapter 23
Editors: Rogers, R. D., Seddon, K. R.
(ACS Symposium Series; No. 902).
Source: orbit
Source-ID: 210454
Research output: Research - peer-review » Article in proceedings – Annual report year: 2005

Supported Ionic Liquid-Phase (SILP) catalysts
General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Jørgensen, B., Riisager, A., Fehrmann, R.
Publication date: 2005
Peer-reviewed: Yes
Event: Poster session presented at Catalysis and Biocatalysis in Green Chemistry, Cambridge, United Kingdom.
Research output: Research - peer-review » Poster – Annual report year: 2005

Supported Liquid Phase Catalysis: An old success with molten salts - a new era with ionic liquids?
General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Contributors: Riisager, A., Rasmussen, S. B., Eriksen, K. M., Fehrmann, R.
Publication date: 2005
Peer-reviewed: Yes
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2005

Thermomorphic phase separation in ionic liquid-organic liquid systems – conductivity and spectroscopic characterization
General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Fehrmann, R., Berg, R. W., van Hal, R., Wasserscheid, P.
Pages: 3052-3058
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 7
ISSN (Print): 1463-9076
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Impact factor 3.906
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Impact factor 4.123
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Continuous fixed-bed gas-phase hydroformylation using supported ionic liquid-phase (SILP) Rh catalysts

Continuous flow gas-phase hydroformylation of propene was performed using novel supported ionic liquid-phase (SILP) catalysts containing immobilized Rh complexes of the biphosphine ligand sulfoxantphos in the ionic liquids 1-n-butyl-3-methylimidazolium hexafluorophosphate and halogen-free 1-n-butyl-3-methylimidazolium n-octylsulfate on silica support. The Rh-sulfoxantphos SILP catalysts proved to be more regioselective than catalysts without ligand and the analogous ionic liquid-free catalysts, giving up to 96% linear product. Furthermore, the performance of the catalysts was generally strongly influenced by the catalyst composition. This is the first report on the use of SILP catalysts for fixed-bed gas-phase hydroformylation.

General information
State: Published
Organisations: Department of Chemistry, Rheinisch-Westfälische Technische Hochschule Aachen
Contributors: Riisager, A., Wasserscheid, P., Van Hal, R., Fehrmann, R.
Pages: 452-455
Publication date: 25 Oct 2003
Peer-reviewed: Yes

Publication information
Journal: Journal of Catalysis
Volume: 219
Issue number: 2
ISSN (Print): 0021-9517
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.99 SJR 2.397 SNIP 1.85
Web of Science (2017): Impact factor 6.759
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.27 SJR 2.451 SNIP 2.142
Web of Science (2016): Impact factor 6.844
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 7.23 SJR 2.668 SNIP 2.177
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.92 SJR 2.688 SNIP 2.233
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.42 SJR 2.553 SNIP 2.091
Web of Science (2013): Impact factor 6.073
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.17 SJR 3.006 SNIP 2.257
Web of Science (2012): Impact factor 5.787
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 6.23 SJR 3.092 SNIP 2.214
Propene and 1-octene hydroformylation with silica-supported, ionic liquid-phase (SILP) Rh-phosphine catalysts in continuous fixed-bed mode

**General information**
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Eriksen, K. M., Wasserscheid, P., Fehrmann, R.
Pages: 149-153
Publication date: 2003
Peer-reviewed: Yes

**Publication information**
Journal: Catalysis Letters
Volume: 90
ISSN (Print): 1011-372X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Propene and 1-octene hydroformylation with silica-supported, ionic liquid-phase (SILP) Rh-phosphine catalysts in continuous fixed-bed mode

Supported ionic liquid-phase (SILP) catalysts were made by immobilizing Rh-monophosphine complexes of bis(m-phenylguanidinium) phenylphosphine 1 and NORBOS 2 ligands in 1-n-butyl-3-methylimidazolium hexafluorophosphate, [BMIM][PF6], on a silica support. The catalysts were active in continuous gas- and liquid-phase hydroformylation of propene and 1-octene, exhibiting TOFs up to 88 h\(^{-1}\) for SILP Rh-2 catalysts, while only low selectivities up to 74% n-aldehyde (n/iso ratio of 2.8) were obtained. This is the first example of continuous fixed-bed liquid-phase hydroformylation using SILP catalysts.

General information
State: Published
Organisations: Department of Chemistry, Rheinisch-Westfälische Technische Hochschule Aachen
Contributors: Riisager, A., Eriksen, K. M., Wasserscheid, P., Fehrmann, R.
Pages: 149-152
Publication date: 2003
Peer-reviewed: Yes

Publication information
Journal: CATALYSIS LETTERS
Volume: 90
Issue number: 3-4
ISSN (Print): 1011-372X
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.43 SJR 0.73 SNIP 0.729
Web of Science (2017): Impact factor 2.911
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.755 SNIP 0.786
Web of Science (2016): Impact factor 2.799
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.27 SJR 0.748 SNIP 0.749
Web of Science (2015): Impact factor 2.294
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.56 SJR 0.89 SNIP 0.928
Web of Science (2014): Impact factor 2.307
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.45 SJR 0.888 SNIP 0.931
Web of Science (2013): Impact factor 2.291
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.35 SJR 1.016 SNIP 0.98
Propene Hydroformylation by Supported Aqueous-phase Rh-NORBOS Catalysts

The gas-phase hydroformylation reaction of propene using supported aqueous-phase (SAP) Rh-NORBOS modified catalysts in a continuous flow reactor has been examined. SAP catalysts supported on six different support materials were made by wet impregnation using solutions of the precursor complex Rh(acac)(CO)(2) and NORBOS ligand. Catalytic performance of silica gel-based catalysts was examined by altering catalyst composition and reaction conditions. Results were compared to analogous TPPTS catalysts and to catalysts supported on alternative support materials, e.g. silica glass, alumina and carbon. Based on these results the aqueous and the homogeneous nature of the SAP catalysts are discussed.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Contributors: Riisager, A., Eriksen, K. M., Hjortkjær, J., Fehrmann, R.
Pages: 259-272
Publication date: 2003
Peer-reviewed: Yes
Biphasic hydroformylation catalysis: Structure and reactivity of immobilized Rh catalysts modified with water-soluble phosphine ligands

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry
Contributors: Riisager, A., Fehrman, R.
Publication date: Mar 2002

Publication information
Original language: English
Source: orbit
Source-ID: 188123
Research output: Research › Ph.D. thesis – Annual report year: 2002

CTAB micelles and the hydroformylation of octene with rhodium/TPPTS catalysts - Evidence for the interaction of TPPTS with micelle surfaces
The addition of cetyltrimethylammonium bromide (CTAB) to TPPTS/rhodium hydroformylation catalysts has a complicated effect on reaction activity and selectivity. In water alone as the solvent, high CTAB concentration leads to the formation of emulsions and reaction selectivity drops. In aqueous alcohol solvents selectivity also drops but the effect appears to be due to the solvent composition. Emulsion formation is minimized and initial reaction activity goes through a maximum at a CTAB/TPPTS ratio of 3. NMR studies show that there is a strong interaction of CTAB and TPPTS in water while the interaction in aqueous methanol appears to be nonspecific.

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Hanson, B. E.
Pages: 195-202
Publication date: 2002
Peer-reviewed: Yes

Publication information
Journal: Journal of molecular catalysis a-chemical
Volume: 189
Issue number: 2
ISSN (Print): 1381-1169
Ratings:
BFI (2019): BFI-level 1
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Web of Science (2017): Impact factor 4.397
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.96 SJR 1.006 SNIP 1.095
Web of Science (2016): Impact factor 4.211
Web of Science (2016): Indexed yes
Metal complex amino acid synths: syntheses, structures and stereoselective reactions of (iminoacetato)cobalt(III) complexes

Amino acid anions (AAO(-)) chelated to cobalt(III) in [(en)(2)Co(AAO)(O3SCF3)(2)] (AA = Gly, Sar, Ala and Glu) were selectively oxidized to their imine derivatives by a new general procedure utilizing PBr3 and N-bromosuccinimide in dmf.
The new iminoacetato complexes, Lambda- and Delta-[(en)(2)Co(O2CCH=NH)][O3SCF3](2), constitute chiral glycine equivalents which can serve as synths for stereoselective alpha-amino acid synthesis. In alkaline EtOH, quantitative addition of CH2(COMe)(2), CH2(CO2Et)(2) or MeCOCH2CO2Et to the imine of the iminoacetate ligand initially produced both diastereomers of the product alpha-amino acid cobalt(III) complexes. However, subsequent crystallization-induced asymmetric transformations in the heterogeneous reaction mixtures led to better than 90% excess of a single diastereomer after five days, and the diastereopure product triflate salts were obtained after recrystallization. Both enantiomers of isotopically substituted (3-C-13, 98%) aspartic acid were produced by facile synthesis from Delta-[(en)(2)Co(O2CCH=NH)][O3SCF3](2) and diethyl (2-C-13) malonate. The new N-methyliminoacetato complex, rac-[(en)(2)Co(OCCCH(=C-2=NMe))[O3SCF3](2), also yielded to imine addition reactions providing a route to the alpha-N-methylamino acid subclass. The molecular structures of the new imine complexes, Lambda-(+578-[(en)(2)Co(O2CCH=NH)][Br2·H2O and rac-[(en)(2)Co(O2CCH=NMMe)[S2O6·1.5H2O, and the diethyl carboxy-aspartate addition product, (LambdaS,D,DeltaR)-[(en)(2)Co(O2CCH(CH(CO2Et)(2))NH2)](ClO4)(2), were determined by X-ray crystallography.

General information
State: Published
Organisations: Australian National University, University of Copenhagen
Pages: 3054-3064
Publication date: 2002
Peer-reviewed: Yes

Publication Information
Journal: Journal of the Chemical Society. Dalton Transactions
Issue number: 15
ISSN (Print): 1472-7773
Ratings:
BFI (2008): BFI-level 1
Web of Science (2002): Indexed yes
Original language: English
DOIs:
10.1039/b202090d
Source: orbit
Source-ID: 194509
Research output: Research - peer-review › Journal article – Annual report year: 2002

Rh/NORBOS Hydroformylation of SAP Catalysts: Structure and Reactivity

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Eriksen, K. M., Fehrmann, R.
Publication date: 2001
Peer-reviewed: No
Event: Poster session presented at 100. Bunsentagung, Stuttgart, Germany. 
Source: orbit
Source-ID: 50559
Research output: Research › Poster – Annual report year: 2001

Structure and Reactivity of Rh/NORBOS Hydroformylation Catalysts

General information
State: Published
Organisations: Department of Chemistry
Contributors: Riisager, A., Eriksen, K. M., Fehrmann, R.
Publication date: 2001
Peer-reviewed: No
Event: Poster session presented at 5th European Congress on Catalysis, Limerick, Ireland.
Source: orbit
Source-ID: 50563
Research output: Research › Poster – Annual report year: 2001
Projects:

**Low-Temperature Small Molecule Transformations**
Piccirilli, L., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Nielsen, M., Supervisor, Department of Chemistry
01/01/2019 → 31/12/2021
Project: PhD

**Enhancing the activity of microporous zeolites for catalytic sugar transformations**
Zhu, P., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Kegnæs, S., Supervisor, Department of Chemistry
01/12/2018 → 30/11/2021
Project: PhD

**Integrated SILP Catalysts - Membrane Separation Reaction Systems**
Marinkovic, J. M., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Fehrmann, R., Supervisor, Department of Chemistry
Garcia Suárez, E. J., Supervisor, Department of Chemistry
Anden EU-finansiering
01/09/2016 → 31/08/2019
Award relations: Integrated SILP Catalysts - Membrane Separation Reaction Systems
Project: PhD

**Katalytisk omdannelse af biomass til flydende brænslser**
Kunov-Kruse, A. J., PhD Student, Department of Chemistry
Fehrmann, R., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Møller, K. B., Examiner, Department of Chemistry
Beato, P., Examiner
Rogers, R. D., Examiner
DTU, Samfinansiering
01/03/2010 → 19/08/2013
Award relations: Katalytisk omdannelse af biomass til flydende brænslser
Project: PhD

**Katalyse og selektiv gasabsorption i ioniske væsker**
Kolding, H., PhD Student, Department of Chemistry
Fehrmann, R., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Berg, R. W., Examiner, Department of Chemistry
Dupont, J., Examiner
Olsen, E., Examiner
Institut stipendie (DTU)
01/12/2011 → 03/06/2015
Award relations: Katalyse og selektiv gasabsorption i ioniske væsker
Project: PhD

**Development of Zeolite Catalysts and Processes for the Selective Conversion of Sugars to Bio-Polymer Monomers**
Tosi, I., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Taarning, E., Supervisor, DTU Executive School of Business
Offentlig finansiering
15/05/2016 → 14/05/2019
Award relations: Development of Zeolite Catalysts and Processes for the Selective Conversion of Sugars to Bio-Polymer Monomers
Project: PhD
**Bifasisk katalyse**

Riisager, A., PhD Student, Department of Chemistry  
Fehrmann, R., Main Supervisor, Department of Chemistry  
Hjortkjær, J., Supervisor, Department of Chemical and Biochemical Engineering  
Tanner, D. A., Examiner, Department of Chemistry  
Andersson, C., Examiner  
Christensen, C. H., Examiner, Department of Chemical and Biochemical Engineering  
Centerfinansieret  
01/04/1999 → 20/09/2002  
Award relations: Bifasisk katalyse  
Project: PhD

**Methanol Carbonylation by SILP Catalysis**

Hanning, C. W., PhD Student, Department of Chemistry  
Fehrmann, R., Main Supervisor, Department of Chemistry  
Riisager, A., Supervisor, Department of Chemistry  
Berg, R. W., Examiner, Department of Chemistry  
Boghosian, S., Examiner  
Vogel, S., Examiner  
Eksternt finansieret  
01/12/2008 → 19/09/2012  
Award relations: Methanol Carbonylation by SILP Catalysis  
Project: PhD

**DeNOx katalysatorer til biomassefyring**

Kristensen, S. B., PhD Student, Department of Chemistry  
Fehrmann, R., Main Supervisor, Department of Chemistry  
Narklit Jensen, J., Supervisor  
Riisager, A., Supervisor, Department of Chemistry  
Jensen, A. D., Examiner, Department of Chemical and Biochemical Engineering  
Bañares, M. A., Examiner  
Odenbrand, I., Examiner  
ErhvervsPhD-ordningen VTU  
01/08/2009 → 21/05/2013  
Award relations: DeNOx katalysatorer til biomassefyring  
Project: PhD

**Bio-chemicals synthesis with ionic liquid technology**

Paolicchi, D., PhD Student, Department of Chemistry  
Riisager, A., Main Supervisor, Department of Chemistry  
Fehrmann, R., Examiner, Department of Chemistry  
Claver, C., Examiner  
Vogel, S., Examiner  
Forskningsrådsfinansiering  
15/03/2012 → 30/09/2016  
Award relations: Bio-chemicals synthesis with ionic liquid technology  
Project: PhD

**Catalytic Routes to Renewable Polymer Building Blocks**

Hansen, T. S., PhD Student, Department of Chemistry  
Riisager, A., Main Supervisor, Department of Chemistry  
Woodley, J., Supervisor, Department of Chemical and Biochemical Engineering  
Clausen, M. H., Examiner, Department of Chemistry  
Bols, M., Examiner  
Leitner, W., Examiner  
DTU-lønnet stipendie  
01/06/2008 → 14/12/2011  
Award relations: Catalytic Routes to Renewable Polymer Building Blocks  
Project: PhD

**Design of sintering stable heterogenous nanoparticle catalysts**

Abildstrøm, J. O., PhD Student, Department of Chemistry
Kegnæs, S., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Harris, P., Examiner, Department of Chemistry
Kolen'ko, Y. V., Examiner
Nedel, S., Examiner
Institut stipendie (DTU) Samf.
15/03/2013 → 15/02/2017
Award relations: Design of sintering stable heterogenous nanoparticle catalysts
Project: PhD

Catalytic Routes to Renewable Chemicals
Mielby, J. J., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Kegnæs, S., Supervisor, Department of Chemistry
Ståhl, K., Examiner, Department of Chemistry
Stakheev, A. Y., Examiner
Herbst, K., Examiner
Institut stipendie (DTU)
15/07/2011 → 24/09/2014
Award relations: Catalytic Routes to Renewable Chemicals
Project: PhD

Alternative Alkali Resistant deNox Technologies
Due-Hansen, J., PhD Student, Department of Chemistry
Fahrmann, R., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Henriksen, N. E., Examiner, Department of Chemistry
Kröcher, O., Examiner
Jensen, J. R., Examiner, Department of Chemical and Biochemical Engineering
Offentlig finansiering
01/06/2007 → 01/09/2010
Award relations: Alternative Alkali Resistant deNox Technologies
Project: PhD

Bio-fuel synthesis with solid acid functionalized catalysis
Poreddy, R., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Jensen, A. D., Supervisor, Department of Chemical and Biochemical Engineering
Ståhl, K., Examiner, Department of Chemistry
Grunwaldt, J., Examiner, Department of Chemical and Biochemical Engineering
Herbst, K., Examiner
Institut, samfinansiering
01/09/2012 → 02/12/2015
Award relations: Bio-fuel synthesis with solid acid functionalized catalysis
Project: PhD

SILP enzyme catalysis technology for upgrading of biomass C5 monomers
Zeuner, B., PhD Student, Technical Information Center of Denmark
Meyer, A. S., Main Supervisor, Department of Biotechnology and Biomedicine
Pinelo, M., Supervisor, Department of Chemical and Biochemical Engineering
Riisager, A., Supervisor, Department of Chemistry
Jergensen, H., Examiner, Riso National Laboratory for Sustainable Energy
Christakopoulos, P., Examiner
Christensen, M. W., Examiner
1/3 FUU, 1/3 inst 1/3 Andet
15/12/2009 → 23/04/2014
Award relations: SILP enzyme catalysis technology for upgrading of biomass C5 monomers
Project: PhD

Sustainable Chemistry for Biomass Utilization
Nielsen, L. B., PhD Student, Department of Chemistry
Tanner, D. A., Main Supervisor, Department of Chemistry
Fristrup, P., Supervisor, Department of Chemistry  
Riisager, A., Examiner, Department of Chemistry  
Moret, M., Examiner  
Pittelkow, M., Examiner  
Institut stipendie (DTU) Samf.  
01/10/2013 → 17/05/2017  
Award relations: Sustainable Chemistry for Biomass Utilization  
Project: PhD

**Continuous Flow Catalysis by Supported Ionic Liquid Phase (SILP) Catalysts**  
Nordvang, E. C., PhD Student, Department of Chemistry  
Fehrmann, R., Main Supervisor, Department of Chemistry  
Riisager, A., Supervisor, Department of Chemistry  
Jensen, A. D., Examiner, Department of Chemical and Biochemical Engineering  
Rasmussen, S. B., Examiner, Department of Chemical and Biochemical Engineering  
Pollington, S. D., Examiner  
Anden EU-finansiering  
01/08/2011 → 25/03/2015  
Award relations: Continuous Flow Catalysis by Supported Ionic Liquid Phase (SILP) Catalysts  
Project: PhD

**Chemicals from Renewables**  
Ståhlberg, T. J. B., PhD Student, Department of Chemistry  
Riisager, A., Main Supervisor, Department of Chemistry  
Tanner, D. A., Examiner, Department of Chemistry  
Rogers, R. D., Examiner  
Taarning, E., Examiner, Department of Chemistry  
Institut stipendie (DTU)  
15/06/2008 → 21/09/2011  
Award relations: Chemicals from Renewables  
Project: PhD

**Bio-Petrochemicals**  
Gorbanev, Y., PhD Student, Department of Chemistry  
Riisager, A., Main Supervisor, Department of Chemistry  
Woodley, J., Supervisor, Department of Chemical and Biochemical Engineering  
Fristrup, P., Examiner, Department of Chemistry  
Grunwaldt, J., Examiner, Department of Chemical and Biochemical Engineering  
Herbst, K., Examiner  
Offentlig finansiering  
01/04/2008 → 08/02/2012  
Award relations: Bio-Petrochemicals  
Project: PhD

**Sustainable catalysis with functional ionic liquids**  
Søndergaard, H., PhD Student, Department of Chemistry  
Riisager, A., Main Supervisor, Department of Chemistry  
Kegnæs, S., Examiner, Department of Chemistry  
Bica, K., Examiner  
Vogel, S., Examiner  
Institut stipendie (DTU) Samf.  
01/11/2009 → 24/06/2013  
Award relations: Sustainable catalysis with functional ionic liquids  
Project: PhD

**Synthesis, Characterization and Evaluation of Tin-containing Zeolites for Biomass Conversion**  
Tolborg, S., PhD Student, Department of Chemistry  
Risager, A., Main Supervisor, Department of Chemistry  
Sádaba, I., Supervisor, Department of Chemistry  
Kegnæs, S., Examiner, Department of Chemistry  
Pedersen, C. M., Examiner  
Sels, B. F., Examiner
selective and efficient synthesis of ethanol from dimethyl ether and syngas
Rasmussen, D. B., PhD Student, Department of Physics
Christensen, J. M., Supervisor, Department of Chemical and Biochemical Engineering
Moses, P. G., Supervisor, Department of Physics
Riisager, A., Supervisor, Department of Chemical Engineering
Rossmeisl, J., Supervisor, Department of Physics
Studt, F., Supervisor, Department of Physics
Jensen, P. A., Examiner, Department of Chemical and Biochemical Engineering
Sehested, J., Examiner
Swang, O., Examiner
1/3 FUU, 1/3 inst 1/3 Andet
15/12/2011 → 30/09/2015
Award relations: selective and efficient synthesis of ethanol from dimethyl ether and syngas
Project: PhD

Renewable Chemistry with ionic liquid-based Catalysis
Malcho, P., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Tanner, D. A., Examiner, Department of Chemistry
Welton, T., Examiner, DTU Executive School of Business
Taarning, E., Examiner
Forskningsrådsfinansiering
01/07/2011 → 30/09/2014
Award relations: Renewable Chemistry with ionic liquid-based Catalysis
Project: PhD

SILP catalysts for alkoxycarbonylation
Khokarale, S. G., PhD Student, Department of Chemistry
Fehrmann, R., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Garcia Suárez, E. J., Supervisor, Department of Chemistry
Tanner, D. A., Examiner, Department of Chemistry
Claver, C., Examiner
Haumann, M., Examiner
Forskningsrådsfinansiering
01/05/2012 → 02/09/2015
Award relations: SILP catalysts for alkoxycarbonylation
Project: PhD

Spectroscopic Investigations of Copper Substituted Zeolite Catalysts
Godiksen, A. L., PhD Student, Department of Chemistry
Mossin, S., Main Supervisor, Department of Chemistry
Rasmussen, S. B., Supervisor, Department of Chemical and Biochemical Engineering
Riisager, A., Examiner, Department of Chemistry
Chiesa, M., Examiner
Wang, F. R., Examiner
Samfinansierede - Virksomhed
01/10/2013 → 24/01/2018
Award relations: Spectroscopic Investigations of Copper Substituted Zeolite Catalysts
Project: PhD

Fabrication of Green Hydrocarbon Fuels via Capture and Electrolysis of CO2
Ebbehøj, S. L., PhD Student, Department of Energy Conversion and Storage
Mogensen, M. B., Main Supervisor, Department of Energy Conversion and Storage
Jensen, S. H., Supervisor, Department of Energy Conversion and Storage
Riisager, A., Supervisor, Department of Chemistry
Hendriksen, P. V., Examiner, Department of Energy Conversion and Storage
Hartvigsen, J. J., Examiner
Bagtø Hansen, J., Examiner
Forskningsrådsfinansiering
01/03/2012 → 13/05/2015
Award relations: Fabrication of Green Hydrocarbon Fuels via Capture and Electrolysis of CO2
Project: PhD

Catalytic Synthesis of Alcoholic Fuels for Transportation from Syngas
Wu, Q., PhD Student, Department of Chemical and Biochemical Engineering
Jensen, A. D., Main Supervisor, Department of Chemical and Biochemical Engineering
Grunwaldt, J., Supervisor, Department of Chemical and Biochemical Engineering
Riisager, A., Examiner, Department of Chemistry
Østberg, M., Examiner, Department of Chemical and Biochemical Engineering
Temel, B., Supervisor
Hinrichsen, K., Examiner
Eksternt finansieret virksomhed
01/01/2010 → 19/03/2013
Award relations: Catalytic Synthesis of Alcoholic Fuels for Transportation from Syngas
Project: PhD

reactor and process design for chem.- enzymatic synthesis of FDA
Fu, W., PhD Student, Department of Chemistry
Woodley, J., Main Supervisor, Department of Chemical and Biochemical Engineering
Riisager, A., Supervisor, Department of Chemistry
Gernaey, K. V., Examiner, Department of Chemical and Biochemical Engineering
Lye, G. J., Examiner
Wiebe, L., Examiner
DTU-lønnet stipendie
01/03/2008 → 18/04/2012
Award relations: reactor and process design for chem.- enzymatic synthesis of FDA
Project: PhD

Catalytic Conversion of Bio-oil to Fuel for Transportation
Mortensen, P. M., PhD Student, Department of Chemical and Biochemical Engineering
Jensen, A. D., Main Supervisor, Department of Chemical and Biochemical Engineering
Grunwaldt, J., Supervisor, Department of Chemical and Biochemical Engineering
Jensen, P. A., Supervisor, Department of Chemical and Biochemical Engineering
Riisager, A., Examiner, Department of Chemistry
Gabrielsen, J., Examiner, Department of Chemical and Biochemical Engineering
Murzin, D., Examiner
1/3 FUU, 1/3 inst 1/3 Andet
15/08/2010 → 23/04/2014
Award relations: Catalytic Conversion of Bio-oil to Fuel for Transportation
Project: PhD

Lignin biomass conversion to fuels and chemicals
Melián Rodríguez, M., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Kegnæs, S., Supervisor, Department of Chemistry
Shunmugavel, S., Supervisor, Department of Chemistry
Duus, J. Ø., Examiner, Department of Chemistry
Gonzales, M. A. B., Examiner
Johannsen, I., Examiner
Institut stipendie (DTU) Samf.
01/06/2013 → 16/06/2016
Award relations: Lignin biomass conversion to fuels and chemicals
Project: PhD

Design of sintering stable heterogenous nanoparticle catalysts
Gallas-Hulin, A., PhD Student, Department of Chemistry
Kegnæs, S., Main Supervisor, Department of Chemistry
Riisager, A., Supervisor, Department of Chemistry
Mossin, S., Examiner, Department of Chemistry
Rasmussen, S. B., Examiner, Department of Chemical and Biochemical Engineering
Wang, F. R., Examiner
Institut stipendie (DTU) Samf.
01/05/2013 → 21/06/2017
Award relations: Design of sintering stable heterogenous nanoparticle catalysts
Project: PhD

Catalytic reactions in Supercritical Fluids
Beier, M. J., PhD Student, Department of Chemical and Biochemical Engineering
Jensen, A. D., Main Supervisor, Department of Chemical and Biochemical Engineering
Grunwaldt, J., Supervisor, Department of Chemical and Biochemical Engineering
Kontogeorgis, G., Supervisor, Department of Chemical and Biochemical Engineering
Riisager, A., Examiner, Department of Chemistry
Herbst, K., Examiner
Muhler, M., Examiner
1/3 DTU-stip, 2/3 FUR/andet
15/02/2008 → 13/04/2011
Award relations: Catalytic reactions in Supercritical Fluids
Project: PhD

Oxidative catalytic upgrading of carbohydrates and derivatives from biomass
Modvig, A. E., PhD Student, Department of Chemistry
Riisager, A., Main Supervisor, Department of Chemistry
Fristrup, P., Supervisor, Department of Chemistry
Kegnæs, S., Examiner, Department of Chemistry
Nielsen, U. G., Examiner
Lugue, R., Examiner
Samfinansieret - Andet
01/05/2014 → 20/09/2017
Award relations: Oxidative catalytic upgrading of carbohydrates and derivatives from biomass
Project: PhD

Selective Hydrogenation of 1,3-butadiene
Garcia Suárez, E. J., Project Participant, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Riisager, A., Project Participant, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
01/12/2014 → 15/01/2016
Keywords: hydrogenation; continuous flow reactions; fixed-bed reactors; palladium; heterogeneous catalysts; metal nanoparticles
Project: Research

FP1306: Valorisation of lignocellulosic biomass side streams for sustainable production of chemicals, materials & fuels using low environmental impact technologies
Scientists are prompted to seek alternative methodologies for the production of materials, fuels and chemicals using low environmental impact technologies and greener methodologies with comparable efficiencies to those currently available in view of the expected resource scarcity and future oil economy. Lignocellulosic residues can constitute a highly promising (and currently largely under-utilised feedstock with a significant potential to be converted into useful end products. However, a joint multidisciplinary effort from several disciplines including (bio)chemistry, biology, (bio)chemical and biological engineering, forest products sciences as well as environmental sciences and experts in economic assessment in liaison with industry is required to appropriately address the efficient transformation of such residues. The main objective of this COST Action will be to develop a solid European multidisciplinary network able to provide a range of innovative alternatives to the valorisation of lignocellulosic residues to chemicals, fuels and materials making use of environmentally sound protocols from.
Garcia Suárez, E. J., Project Participant, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Riisager, A., Project Participant, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Project ID: FP1306
14/05/2014 → 13/05/2018
Keywords: Valorisation of Lignocellulosic Biomass Residues, Forest Products, Biorefinery
Collaborators: EU COST Office
Project: Research
Inorganic Catalysis
Multidisciplinary investigations of structure and catalytic activity of inorganic catalysts and model systems. In collaboration with ICAT.

Activities:

18th Nordic Symposium on Catalysis
Period: 26 Aug 2018 → 28 Aug 2018
Anders Riisager (Organizer)
Susanne Mossin (Organizer)
Søren Kegnæs (Organizer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Center for Hyperpolarization in Magnetic Resonance
Degree of recognition: International

Related event
18th Nordic Symposium on Catalysis
26/08/2018 → 28/08/2018
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference