Abstract Listing

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414428: Chymotrypsin-catalyzed transesterification in ionic liquids and ionic liquid/supercritical carbon dioxide

IEC 0 [414428]: Chymotrypsin-catalyzed transesterification in ionic liquids and ionic liquid/supercritical carbon dioxide

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-19*

Abstract

Ionic liquids are molten organic salts at or near room temperature, which have been shown to be useful media for many reactions. With the possibility of incorporating another "green" solvent, supercritical carbon dioxide (SC-CO_2), into the reaction/extraction processing scheme, further utility may be achieved. To date, there have been no reports in the literature of reactions in ionic liquids catalyzed by isolated enzymes. We have examined the transesterification reaction of *N*-acetyl-L-phenylalanine ethyl ester with 1-propanol catalyzed by chymotrypsin in the ionic liquids 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF_6]) and 1-octyl-3-methylimidazolium hexafluorophosphate ([omim][PF_6]). In addition, this reaction was studied with SC-CO_2 included as a miscible co-solvent. Protease-catalyzed reactions (amidation, esterification, and transesterification) proceed in aqueous-organic and nearly-anhydrous organic solvents with rates greatly dependent on solvent polarity, solvent water activity, and enzyme support properties. The activity of chymotrypsin was studied to determine whether the trends observed with this enzyme in conventional organic solvents hold for the novel environment provided by ionic liquids. Chymotrypsin freeze-dried with K_2HPO_4, or with K_2HPO_4 and poly(ethylene glycol), demonstrated no activity in [bmim][PF_6] or [omim][PF_6] at very low water concentrations, but low transesterification rates were observed with the ionic liquids containing up to 2.0% water (vol/vol). However, the physical complexation of the enzyme with poly(ethylene glycol) did not stimulate activity in the ionic liquids, unlike that observed in acetonitrile, hexane, or isooctane. These results indicate that [bmim][PF_6] and [omim][PF_6] provide

an environment more similar to polar solvents such acetonitrile than nonpolar solvents, resulting in lower activities than that which can be achieved in very nonpolar solvents. Inclusion of supercritical carbon dioxide in the reaction medium increased enzyme activity substantially, indicating that the combined ionic liquid/SC-CO_2 serves as a better medium than either fluid alone.

419434: Green synthesis: Ionic liquids and cross coupling reactions

IEC 0 [419434]: Green synthesis: Ionic liquids and cross coupling reactions

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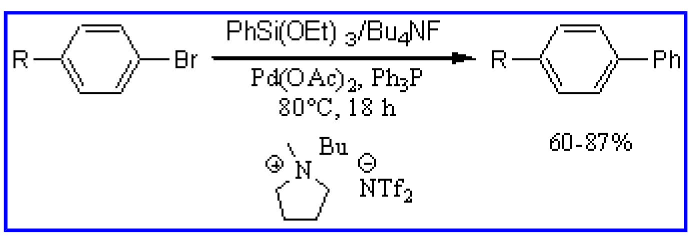
ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II*
Invited: *N*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-24*

Abstract

As pressures continue to mount to make synthesis more environmentally compatible as well as more practical and cost-effective, new techniques for achieving these goals continue to be developed. One of the more interesting recent developments has been the use of ionic liquids as replacements for conventional organic solvents. These ionic liquids have the interesting ability to dissolve both organic and inorganic materials and thus have already found application as a reaction media for transition metal catalyzed reactions such as hydrogenations and the Heck reaction. The present research reports on the use of ionic liquids and various palladium catalysts as stable and recyclable reaction systems for a variety of Stille and DeShong coupling reactions.



419511: Bioprocess applications of ionic liquids: Opportunities and challenges

IEC 0 [419511]: Bioprocess applications of ionic liquids: Opportunities and challenges

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *Powerpoint presentation facilities*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-19*

Abstract

Operations employing mixtures of aqueous and organic phases are used throughout the bioprocessing industries. These include antibiotic recovery by solvent extraction and the synthesis of pharmaceutical intermediates using whole cell or isolated enzyme biocatalysts. In addition to their known safety and environmental problems organic solvents also damage bacterial cell walls and the tertiary structure of enzymes. Recent work in our laboratory, and elsewhere, has established that ionic liquids can replace organic solvents for the regioselective hydration of aromatic dinitriles using a whole cell Rhodococcus catalyst and the thermolysin catalysed synthesis of Z-aspartame. In both cases use of ionic liquid phases led to enhancements in catalyst stability. This paper will assess the opportunities for using ionic liquids in biocatalytic processes and outline key research that remains to be addressed. In particular the possibility of altering the selectivity of enzyme catalysts through the rational modification of ionic liquid media will be described.

423086: Biphasic hydroformylation of 1-octene using ionic liquids as catalyst phase

IEC 0 [423086]: Biphasic hydroformylation of 1-octene using ionic liquids as catalyst phase

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ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-19*

Abstract

In the Ruhrchemie-Rhône-Poulenc-process, Rh-catalysed hydroformylation is technically realised in a biphasic reaction mode using an aqueous catalyst phase. Unfortunately, this process is limited to C_2-

C_5-olefins due to the low water solubility of higher olefins. As alternative polar medium for biphasic hydroformylation, Chauvin et al. introduced ionic liquids. However, none of the tested catalystic systems (IL, Rh-precursor + PPh_3 or sulfonated triaryl phophines) allowed a combination of high activity, complete retention of the catalyst and high selectivity for the desired linear hydroformylation product. In our contribution we present several examples for the use of ionic liquids in biphasic, highly active and highly selective 1-octene hydroformylation without detectable catalyst leaching. Two general systems will be discussed in detail. 1) Pt-catalysed hydroformylation in chlorostannate ionic liquids. 2) Rh-catalysed hydroformylation in hexafluorophosphate ionic liquids using cationic ligand systems such as e.g. cobaltoceniumdiphosphines and diphosphines with a guanidinium modified xanthene backbone.

438650: Reactivity of lignocellulosic biomass derivatives in ionic liquids

IEC 0 [438650]: Reactivity of lignocellulosic biomass derivatives in ionic liquids

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Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II*
Invited: *Y*
Preferred Presentation Format: *Oral*
Consider for Sci-Mix: *N*
Special Equipment Needs: *overhead projector/microphone*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-19*

Abstract

The processing of lignocellulosic biomass into a series of distinct chemicals poses many challenges due to the high degree of structural complexity and high oxygen-to-carbon ratio of both the carbohydrate fraction and the lignins. A direct consequence of this is that well-established catalytic chemistry that is commonly applied to the chemical conversion of petrochemicals, does not always apply to the processing of lignocellulosic feedstocks. Most often, aqueous or aqueous-organic solvent systems are used wherein the organic phase usually consists of solvents like e.g. DMF, DMSO or pyridine, in order to dissolve the highly polar carbohydrates. On the other hand, lignins are notoriously difficult materials to process also, because they tend to not dissolve at all in traditional solvents. We have started with an exploratory study of ionic liquids as novel solvent systems for the chemical conversion of carbohydrates and lignins, and this presentation will focus on our progress.

442338: Green chemistry, the carbohydrate economy, and ionic liquids: Compatible goals, compatible chemistries?

IEC 0 [442338]: Green chemistry, the carbohydrate economy, and ionic liquids: Compatible goals, compatible chemistries?

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Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II*
Invited: *Y*
Preferred Presentation Format: *OralOnly*
Consider for Sci-Mix: *N*
Conforms to Bylaw 6: *Y*
Last Modified: *2000-11-24*

Abstract
Green Chemistry focuses on interdisciplinary activities related to waste minimization, the development of green manufacturing processes, and the minimization of environmental and manufacturing costs. Increasingly, new technologies, new laws, and public awareness are ushering in plant matter as the new material base for the new millennium, the so-called “carbohydrate economy.” Carbohydrates can be converted into chemicals, energy, textiles, building materials, paper, and many other industrial products, but a major barrier to utilization is the availability of cost effective, clean separation and processing technologies. The nascent field of ionic liquids as solvents offers a unique opportunity to investigate such new technologies from several perspectives having the same overall objectives. This presentation will discuss our new efforts to apply ionic liquids to the development of new products from sugar cane.

445127: Intermission

0 [445127]: Intermission

ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II* ***Preferred Presentation Format:*** *Break*
Consider for Sci-Mix:
Last Modified: *2000-11-24*

Abstract: Abstract text not available.

445128: Discussion

0 [445128]: Discussion

ACCEPTED
Topic Selection: *Green (or Greener) Industrial Applications of Neoteric Solvents: Ionic and Supercritical Fluids: Catalysis II* ***Preferred Presentation Format:*** *Break*

Consider for Sci-Mix:
Last Modified: *2000-11-24*

Abstract: Abstract text not available.