Accepted Manuscript

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PII:	S0021-9797(16)31069-4
DOI:	http://dx.doi.org/10.1016/j.jcis.2016.12.063
Reference:	YJCIS 21897
To appear in:	Journal of Colloid and Interface Science
Received Date:	25 November 2016
Accepted Date:	26 December 2016



Please cite this article as: A. Cognigni, S. Kampichler, K. Bica, Surface-active ionic liquids in catalysis: Impact of structure and concentration on the aerobic oxidation of octanol in water, *Journal of Colloid and Interface Science* (2016), doi: http://dx.doi.org/10.1016/j.jcis.2016.12.063

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Surface-active ionic liquids in catalysis: Impact of structure and concentration on the aerobic oxidation of octanol in water

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Abstract

We present design and synthesis of surface-active ionic liquids for the application in micellar catalysis. A series of 1-methyl-3-dodecylimidazolium based ionic liquids with variable core structures including dicationic and zwitterionic ones was synthesized and characterized. These surface-active ionic liquids where applied in the aerobic oxidation of aliphatic alcohols to carbonyl compounds. A strong dependence on the ionic liquid concentration and structure was identified, which is in accordance with the concepts of micellar catalysis. Optimum conditions for the oxidation of 1-octanol could be identified, and the use of surface-active ionic liquids strongly improved the reaction performance compared to pure water. Under optimized conditions, it was possible to isolate up to 75% of octanoic acid using only small amounts of surface-active ionic liquid in a 0.05 mM solution in water without further ligands.

Keywords: micellar catalysis, water, surfactants, ionic liquids, aerobic oxidation, Palladium *2010 MSC:* 00-01, 99-00

Introduction

Solvent consumption accounts for a relevant part of the overall environmental impact of a chemical process. Replacing traditional volatile organic solvents with more benign ones such as water can be a key step towards the development of sustainable processes, although problems with substrate solubility may exist.[1] The addition of commercially available surfactants provides a powerful tool to overcome the solubility issue of many organic substrates in water, as the formation of aggregates in water enables the solubilization of reaction mixtures in water. Micelles or higher aggregates have the capability to drastically alter

Preprint submitted to Journal of Colloid and Interface Science

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