

Ionic Liquids par excellence

PUBLICATIONS:

Kalb R. et al, Carbonate based ionic liquid synthesis (CBILS®): thermodynamic analysis, Phys. Chem. Chem. Phys., 2016,18, 31904-31913
DOI: 10.1039/C6CP06594E

Abstract

Within the last decade the Carbonate Based Ionic liquid Synthesis (CBILS®) has developed towards a widely applicable, greener and halogen free process for the industrial production of ionic liquids. A large number of diverse starting materials have been screened experimentally, to explore the structural limits of the core reaction step, which is the quaternization of nitrogen, phosphor or sulfur based nucleophiles with carbonic acid dialkyl or diaryl esters to the corresponding quaternary alkyl- or arylcarbonates. In order to overcome the large experimental effort of empirical screening, a practical method based on quantum-chemical calculation has been developed for an assessment of feasibility of chemical reactions. This method has been successfully tested with 16 typical CBILS® reactions by calculation of their thermodynamic functions. Thermodynamic equilibrium constants as a measure for the practical yield of the CBILS® reactions at 298 K and 393 K have been determined for both the gaseous state and the liquid state. The method has been evaluated by comparison of the theoretical results with experimental data and it can be considered as the powerful tool to reduce “trial and failure” for the industrial application of the CBILS® process.

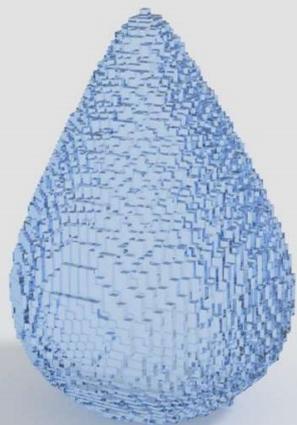
<http://pubs.rsc.org/en/Content/ArticleLanding/2016/CP/C6CP06594E#!divAbstract>

Kalb R. et al, Carbonate Based Ionic Liquid Synthesis (CBILS®): development of the continuous flow method for preparation of ultra-pure ionic liquids, React. Chem. Eng., 2017,2, 432-436
DOI: 10.1039/C7RE00028F

Abstract

Carbonate Based Ionic Liquid Synthesis (CBILS®) is one of the most advanced commercialized processes for greener and halide-free technical synthesis of ionic liquids (ILs). To meet the increasing demand for high purity ILs, a continuous flow method with an improved space-time yield was developed. The quality of resulting ILs and IL-intermediates was confirmed to be ultra-high, by traditional analytical methods as well as by extremely sensitive combustion and solution calorimetry techniques.

<http://pubs.rsc.org/en/Content/ArticleLanding/2017/RE/C7RE00028F#!divAbstract>



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R. E. Whiteside et al, **Selective monoalkylation of p-tert-butylcalix-[4]-arene in a methyl carbonate ionic liquid**, Chem Commun (Camb). 2018 Oct 23;54(85):12037-12040. doi: 10.1039/c8cc05566a

Abstract

Methyl carbonate ionic liquids are shown to readily mono-deprotonate p-tert-butylcalix-[4]-arenes initiating the formation of an organic mono-anionic p-tert-butylcalix-[4]-arate salt, methanol and carbon dioxide. These calix-[4]-arate salts have been successfully used in alkylation reactions with dialkyl sulfates and alkyl halides to form a mono-alkylated single product with high yield. This method avoids the common use of alkali metal bases such as caesium fluoride hence providing a safer and more selective synthetic route.

<https://pubs.rsc.org/en/content/articlelanding/2018/cc/c8cc05566a#!divAbstract>