2006
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NUMBER 9

ChemFiles

ALDRICH
Fluka

Ionic Liquids

CELLIONICS™

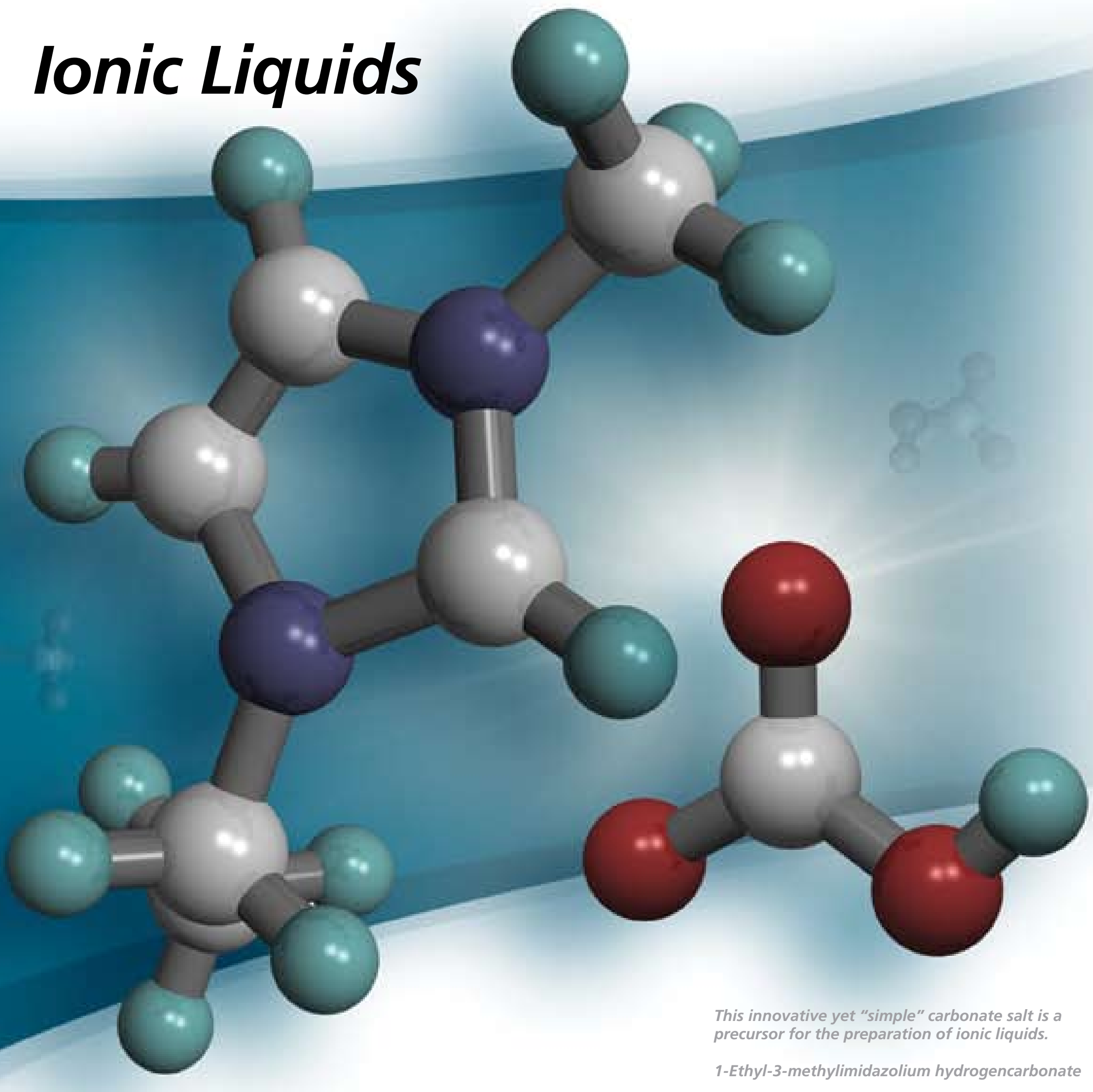
NEW BASIONICS™

CBILS©

DIBUTYLPHOSPHATE AND “NATURAL” IONIC LIQUIDS

TRIOCTYLMETHYL-AMMONIUM THIOSALICYLATE (TOMATS)

NITRILE (CYANO) FUNCTIONALIZED IONIC LIQUIDS



This innovative yet “simple” carbonate salt is a precursor for the preparation of ionic liquids.

1-Ethyl-3-methylimidazolium hydrogencarbonate

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Introduction

As a recent *Chemical and Engineering News* headline illustrated, the use of ionic liquids is no longer exclusive to academic labs.[1] The number of literature citations regarding industrial applications of ionic liquids is increasing. Among the best-known examples are the successful licensing of the BASIL™ process[2] by BASF to a variety of companies and the use of ionic liquids by Degussa as performance additives in pigment pastes.[3] Another example of an industrial application exhibiting high potential is the dissolution of cellulose. In collaboration with BASF, Sigma-Aldrich is proud to present CELLIONICs™, the first commercially available, ready-to-use, ionic liquid solutions of cellulose! Finally, ionic liquids have made a longtime dream of mechanical engineering come true: Linde AG has developed the ionic compressor, a machine that allows compressing gases at constant temperatures, i.e. isothermal compression.[4] The operating fluid in the compressor is an ionic liquid, which was developed by the Austrian company proionic GmbH.

With these recent success stories, ionic liquid technologies are certain to broaden in the coming years. At Sigma-Aldrich we are committed to being your preferred supplier of ionic liquids. Please visit **sigma-aldrich.com/ionicliquids** for a comprehensive listing of products. If you cannot find a product, we welcome your input and will use it to broaden our product range even further. Please contact us at **dweibel@europe.sial.com** with your suggestion!

References: (1) *Chem. Eng. News* **2006**, *84*, 14. (2) *ChemFiles* Vol. 5 No. 6. (3) Weyershausen, B.; Lehmann, K. *Green Chem.* **2005**, *7*, 15. (4) Linde Technology – Reports on Science and Technology, January 2006, available as PDF from www.linde.com.

About Our Cover

The cover illustration depicts 1-ethyl-3-methylimidazolium (EMIM) hydrogencarbonate, which was developed by the Austrian company **proionic GmbH**. This innovative yet "simple" carbonate salt is a precursor for the preparation of ionic liquids. Treatment of this salt with any Brønsted acid quantitatively yields the desired ionic liquid, being composed of the EMIM cation and the conjugate anion of the added Brønsted acid. The water and carbon dioxide by-products are readily removed from the newly formed ionic liquid.

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Cellionics™

Solutions of Cellulose in Ionic Liquids

Dr. Matthias Maase, Dr. Klemens Massonne, Dr. Eric Uerdingen, Dr. Uwe Vagt, BASF Aktiengesellschaft, 67056 Ludwigshafen, Germany, www.basionics.com

At an estimated volume of ~700 billion tons, cellulose is the earth's most widespread natural organic substance, making it an important biorenewable resource. Of the 40 billion tons nature renews every year, only 0.2 billion tons are used as feedstock for further processing.

Intensive exploitation of cellulose as a biorenewable feedstock has to date been prevented by the lack of a suitable solvent that can be used in the chemical processes. Robin Rogers and co-workers at the University of Alabama have found that solutions of cellulose can now be produced for the first time at useful concentrations using ionic liquids as solvents.[1] This new technology opens up substantial potential for cellulose processing and manufacturing of new cellulose-based materials.

Currently, making cellulose fiber by the dissolving pulp method requires the use, and subsequent disposal of, tremendous volumes of various chemical additives. Approximately 600,000 metric tons of carbon disulfide (CS_2) are consumed each year for this application. For each ton of cellulose fiber produced, there are more than two tons of waste substances. During the process, major volumes of waste water are produced that must be treated. These processes can be greatly simplified by the use of ionic liquid solvents, which are nearly entirely recycled. This can clearly reduce the amount of auxiliaries needed (**Figure 1**).

BASF and the Institute for Textile Chemistry and Chemical Fibers (ITCF) in Denkendorf are jointly investigating the properties of fibers spun from an ionic liquid solution of cellulose in pilot plant manufacturing. The fibers obtained show a smooth surface with a circular cross-section (**Figure 2**).

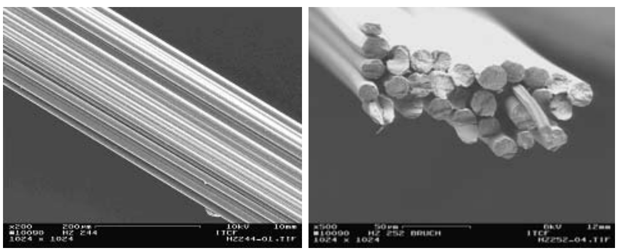


Figure 2: SEM micrographs of cellulose fibers spun from an ionic liquid solution.

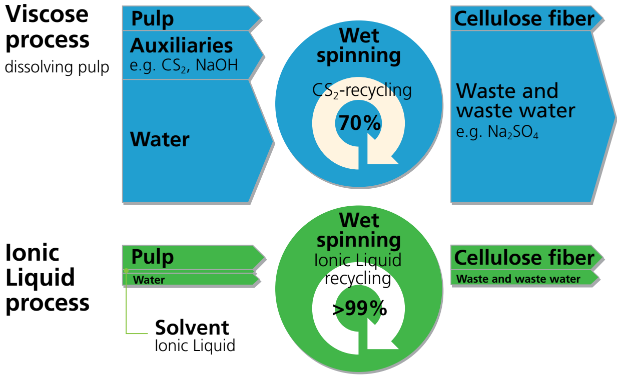


Figure 1: Current viscose process[2] compared to an ionic liquid-based solvent process. The new ionic liquid process does not need CS_2 as an auxiliary and offers the potential to significantly decrease the waste-per-ton cellulose fiber produced.

Partnering with the University of Alabama, BASF has licensed the exclusive use of various ionic liquid technologies in the field of dissolution and processing of cellulose.[3] BASF intends to tap the potential of this fascinating application fast and purposefully in co-operations together with customers and research partners.[4]

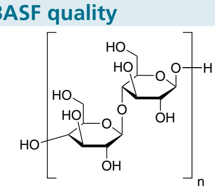
Cellulose in ionic liquids gives real physical solutions. The crystallinity of the cellulosic raw material fully disappears on dissolving it in the ionic liquid. BASIONIC™ BC 01 can dissolve up to 25 wt % of cellulose. The cellulose solutions show excellent long-term stability even at elevated temperatures without a significant decrease of the average degree of polymerization (DP). They do not contain gel particles and are air-stable.

BASF has now launched a series of solutions of cellulose in ionic liquids under the brand name CELLIONIC™. These are 5 wt % solutions of cellulose in EMIM acetate (BASIONIC™ BC 01) with cellulose of different DPs. The celluloses used in the CELLIONICs™ cover DPs of approximately 350, 680, and 1100. The cellulose raw material is provided by the Cellulose Fibers Business of Weyerhaeuser Company. Lab-scale quantities (100 g and 1 kg packages) will be available from Sigma-Aldrich in early 2007.

References: (1) WO 2003 029329; Swatloski, R. P.; Spear, S. K.; Holbrey, J. D.; Rogers, R. D. *J. Am. Chem. Soc.* **2002**, *124*, 4974. (2) Albrecht, W.; Külter, H.; Wulfhorst, B. *Chemiefasern/Textilindustrie* **1990**, *92*, 1046. (3) BASF press release, P-05-519, November 14, 2005. (4) BASF press release, P-06-367, August 29, 2006.

CELLIONIC BCW 700 – Cellulose solution, 5% in 1-ethyl-3-methylimidazolium acetate, BASF quality NEW

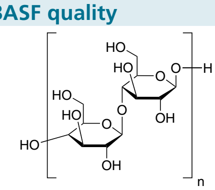
Weyerhaeuser cellulose HW-14917-40-2 with DP of approximately 680



672157-100G	100 g
672157-1KG	1 kg

CELLIONIC BCW 1100 – Cellulose solution, 5% in 1-ethyl-3-methylimidazolium acetate, BASF quality NEW

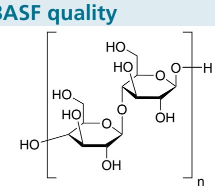
Weyerhaeuser cellulose HW-14917-40-1 with DP of approximately 1100



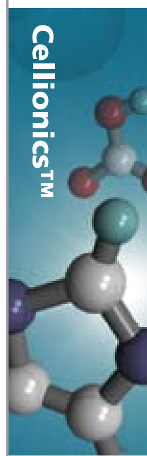
672041-100G	100 g
672041-1KG	1 kg

CELLIONIC BCW 400 – Cellulose solution, 5% in 1-ethyl-3-methylimidazolium acetate, BASF quality NEW

Weyerhaeuser cellulose EM-14911-11 with DP of approximately 350



672270-100G	100 g
672270-1KG	1 kg



New BASIONICS™

Under the trade name BASIONICS™, BASF offers a portfolio of ionic liquids. Within the BASIONICS™ portfolio, the ionic liquids can be classified as: (1) standard, (2) acidic, (3) basic, (4) liquid at room temperature, and (5) low viscosity products, opening up a wide variety of potential applications. Driven by customer demand, the living portfolio of the BASIONICS™ has been extended to include five exciting new products. The BASIONICS™ portfolio is exclusively available from Sigma-Aldrich in kilogram scale.

BASIONIC™ FS 65 Choline salicylate

Choline salicylate (BASIONIC™ FS 65) is a low-melting ionic liquid (36–38 °C). Representative non-solvent applications described in the patent literature include:

- Use as drilling fluids[1]
- Additives for pharmaceutical products[2]
- Additives for the polymerization of polyoxymethylene copolymers[3]

Molar Mass		**Melting Point (°C)**
241.48		36–38
Viscosity at rt (mPa·s)	**Viscosity at 80 °C (mPa·s)**	**Density at rt (g/cm³)**
	89.5	
Density at 80 °C (g/cm³)	**Electrochemical Window (V)**	**Electric Conductivity (μS/cm)**
1.1467		
Heat Conductivity (W/(m·K))	**Heat Capacity (J/(g·K))**	**Flashpoint (°C)**
		183
Flammability Point (°C)	**Solubility in Water**	
325		

BASIONIC™ FS 85 Choline Acetate

Choline acetate (BASIONIC™ FS 85) is an interesting reaction medium for biocatalysis. In the chloroperoxidase-catalyzed conversion of methyl phenyl sulfides to the corresponding sulfoxides, it acts as a suitable co-solvent, leading to satisfactory yields and very good enantioselectivities. In addition, over-oxidation of the sulfoxide to the sulfone is not observed.[4]

Molar Mass		**Melting Point (°C)**
163.21		85
Viscosity at rt (mPa·s)	**Viscosity at 80 °C (mPa·s)**	**Density at rt (g/cm³)**
	89.5	
Density at 80 °C (g/cm³)	**Electrochemical Window (V)**	**Electric Conductivity (μS/cm)**
	−2.5/+1.2	
Heat Conductivity (W/(m·K))	**Heat Capacity (J/(g·K))**	**Flashpoint (°C)**
		140
Flammability Point (°C)	**Solubility in Water**	
285		

BASIONIC™ FS 01 Tris(2-hydroxyethyl)methyl-ammonium methylsulfate

BASIONIC™ FS 01 is a RTIL (**R**oom **T**emperature **I**onic **L**iquid) remaining as a liquid below 20 °C. Furthermore, BASIONIC™ FS 01 is remarkable in view of its toxicological and ecotoxicological profile.

Table 1: BASIONIC™ FS 01, an ecologically friendly RTIL with a complete toxicological data set.

	BMIM Cl*	EMIM $EtOSO_3$**	MTEOA $MeOSO_3$***
Acute oral toxicity	Toxic	Not harmful	Not harmful
Skin irritation	Irritant	Non-irritant	Non-irritant
Eye irritation	Irritant	Non-irritant	Non-irritant
Sensitization	Non-sensitizing	Non-sensitizing	Non-sensitizing
Mutagenicity	Non-mutagenic	Non-mutagenic	Non-mutagenic
Biological degradability	Not readily degradable	Not readily degradable	Readily biodegradable
Toxicity to *daphniae*	Acutely toxic	Not acutely harmful	Not acutely harmful
Toxicity to fish	Not acutely harmful	–	Not acutely harmful

*BMIM Cl = 1-Butyl-3-methylimidazolium chloride
**EMIM $EtOSO_3$ = 1-Ethyl-3-methylimidazolium ethylsulfate
***MTEOA $MeOSO_3$ = Tris(2-hydroxyethyl)methylammonium methylsulfate

Molar Mass		**Melting Point (°C)**
275.32		< −20
Viscosity at rt (mPa·s)	**Viscosity at 80 °C (mPas)**	**Density at rt (g/cm³)**
686	53.4	1.34
Density at 80 °C (g/cm³)	**Electrochemical Window (V)**	**Electric Conductivity (μS/cm)**
1.31		
Heat Conductivity (W/(m·K))	**Heat Capacity (J/(g·K))**	**Flashpoint (°C)**
		198
Flammability Point (°C)	**Solubility in Water**	
380	∞	

BASIONIC™ ST 33 1,2,4-Trimethylpyrazolium methylsulfate

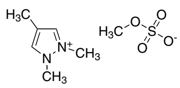
1,2,4-Trimethylpyrazolium methylsulfate displays a high thermal stability (DSC decomposition onset: 350 °C). Therefore, it is suitable for reactions that require high temperatures such as Diels-Alder reactions. Furthermore, it has potential applications as a thermofluid.

Molar Mass		**Melting Point °C**
222.29		33–34
Viscosity (at rt mPas)	**Viscosity (at 80 °C mPas)**	**Density (at rt g/cm³)**
	27.2	
Density (at 80 °C g/cm³)	**Electrochemical (Window V)**	**Electric Conductivity (µS/cm)**
1.250	−1.7/+2.0	
Heat Conductivity (W/(m·K))	**Heat Capacity (J/(g·K))**	**Flashpoint (°C)**
		142
Flammability Point (°C)	**Solubility in Water**	
420	∞	

References: (1) Haliburton Energy Services, USA, US 643685. (2) Hebei Normal University, Peoples Republic of China, CN 1651089. (3) Asahi Chemicals. Inc, Japan, JP 2000119357. (4) Chiappe, C.; Neri, L.; Pieraccini, D. *Tetrahedron Lett.* **2006**, *47*, 5089.

1,2,4-Trimethylpyrazolium methylsulfate, BASF quality, ≥95% NEW

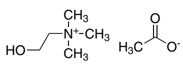
$C_7H_{14}N_2O_4S$
FW: 222.26
[*856614-13-6*]



56595-100G	100 g
56595-1KG	1 kg

Choline acetate, BASF quality, ≥95% NEW

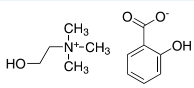
$C_7H_{17}NO_3$
FW: 163.21
[*14586-35-7*]



73215-100G	100 g
73215-1KG	1 kg

Choline salicylate, BASF quality, ≥95% NEW

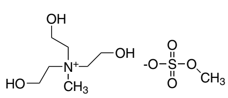
$C_{12}H_{19}NO_4$
FW: 241.28
[*2016-36-6*]



43785-100G	100 g
43785-1KG	1 kg

Tris(2-hydroxyethyl)methylammonium methylsulfate, BASF quality, ≥95% NEW

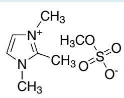
$C_8H_{21}NO_7S$
FW: 275.32
[*29463-06-7*]



91198-100G	100 g
91198-1KG	1 kg

1,2,3-Trimethylimidazolium methylsulfate, BASF quality, ≥95%

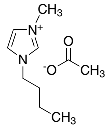
$C_7H_{14}N_2O_4S$
FW: 222.26
[*65086-12-6*]



50365-100G-F	100 g
50365-1KG-F	1 kg

1-Butyl-3-methylimidazolium acetate, BASF quality, ≥95%

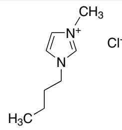
$C_{10}H_{18}N_2O_2$
FW: 198.26
[*284049-75-8*]



39952-100G-F	100 g
39952-1KG-F	1 kg

1-Butyl-3-methylimidazolium chloride, BASF quality, ≥95%

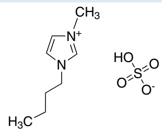
$C_8H_{15}ClN_2$
FW: 174.67
[*79917-90-1*]



38899-100G-F	100 g
38899-1KG-F	1 kg

1-Butyl-3-methylimidazolium hydrogensulfate, BASF quality, ≥95%

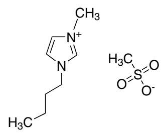
$C_8H_{16}N_2O_4S$
FW: 236.29
[*262297-13-2*]



57457-100G-F	100 g
57457-1KG-F	1 kg

1-Butyl-3-methylimidazolium methanesulfonate, BASF quality, ≥95%

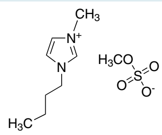
$C_9H_{18}N_2O_3S$
FW: 234.32
[*342789-81-5*]



30881-100G-F	100 g
30881-1KG-F	1 kg

1-Butyl-3-methylimidazolium methylsulfate BASF quality, ≥95%

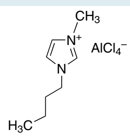
$C_9H_{18}N_2O_4S$
FW: 250.32
[*401788-98-5*]



53177-100G-F	100 g
53177-1KG-F	1 kg

1-Butyl-3-methylimidazolium tetrachloroaluminate, BASF quality, ≥95%

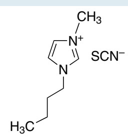
$C_8H_{15}AlCl_4N_2$
FW: 308.01
[*80432-09-3*]



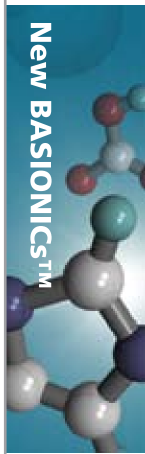
55292-100G-F	100 g
55292-1KG-F	1 kg

1-Butyl-3-methylimidazolium thiocyanate, BASF quality, ≥95%

$C_9H_{15}N_3S$
FW: 197.30
[*344790-87-0*]

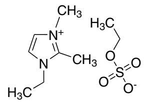


42254-100G-F	100 g
42254-1KG-F	1 kg



1-Ethyl-2,3-dimethylimidazolium ethylsulfate BASF quality, ≥95%

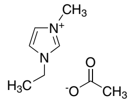
$C_9H_{18}N_2O_4S$
FW: 250.32
[*516474-08-1*]



05338-100G-F	100 g
05338-1KG-F	1 kg

1-Ethyl-3-methylimidazolium acetate, BASF quality, ≥90%

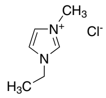
$C_8H_{14}N_2O_2$
FW: 170.21
[*143314-17-4*]



51053-100G-F	100 g
51053-1KG-F	1 kg

1-Ethyl-3-methylimidazolium chloride, BASF quality, ≥95%

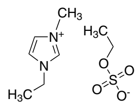
$C_6H_{11}ClN_2$
FW: 146.62
[*65039-09-0*]



30764-100G-F	100 g
30764-1KG-F	1 kg

1-Ethyl-3-methylimidazolium ethylsulfate, BASF quality, ≥95%

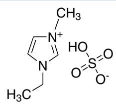
$C_8H_{16}N_2O_4S$
FW: 236.29
[*342573-75-5*]



51682-100G-F	100 g
51682-1KG-F	1 kg

1-Ethyl-3-methylimidazolium hydrogensulfate, BASF quality, ≥95%

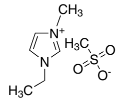
$C_6H_{12}N_2O_4S$
FW: 208.24
[*412009-61-1*]



56486-100G-F	100 g
56486-1KG-F	1 kg

1-Ethyl-3-methylimidazolium methanesulfonate, BASF quality, ≥95%

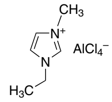
$C_7H_{14}N_2O_3S$
FW: 206.26
[*145022-45-3*]



29164-100G-F	100 g
29164-1KG-F	1 kg

1-Ethyl-3-methylimidazolium tetrachloroaluminate, BASF quality, ≥95%

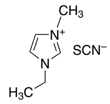
$C_6H_{11}AlCl_4N_2$
FW: 279.96
[*80432-05-9*]



51059-100G-F	100 g
51059-1KG-F	1 kg

1-Ethyl-3-methylimidazolium thiocyanate, BASF quality, ≥95%

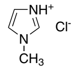
$C_7H_{11}N_3S$
FW: 169.25
[*331717-63-6*]



43437-100G-F	100 g
43437-1KG-F	1 kg

1-Methylimidazolium chloride, BASF quality, ≥95%

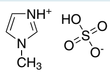
$C_4H_6N_2 \cdot HCl$
FW: 118.56
[*35487-17-3*]



40477-100G-F	100 g
40477-1KG-F	1 kg

1-Methylimidazolium hydrogensulfate, BASF quality, ≥95%

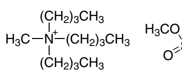
$C_4H_6N_2 \cdot H_2SO_4$
FW: 180.18
[*681281-87-8*]



59760-100G-F	100 g
59760-1KG-F	1 kg

Tributylmethylammonium methylsulfate, BASF quality, ≥95%

$C_{14}H_{33}NO_4S$
FW: 311.48
[*13106-24-6*]



38938-100G-F	100 g
38938-1KG-F	1 kg

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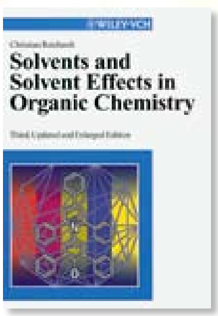
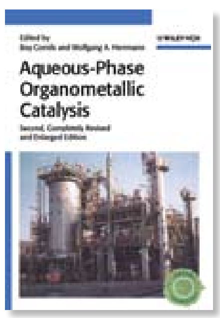


Solvents and Solvent Effects in Organic Chemistry

C. Reichardt, Wiley, 2003, 654 pp., Hardcover. In most cases, every chemist must deal with solvent effects, whether voluntarily or otherwise. Since its publication, this has been the standard reference on all topics related to solvents and solvent effects in organic chemistry. Christian Reichardt provides reliable information on the subject, allowing chemists to understand and effectively use these phenomena. The 3rd Edition, updated and enlarged with 35% more content, includes current developments about ionic liquids.

Z553492-1EA



Aqueous-Phase Organometallic Catalysis: Concepts and Applications, 2nd Edition

B. Cornils and W. A. Herrmann, Wiley, 2004, 780 pp., Hardcover. This is a method which facilitates separation in an efficient and "green" way. Time, waste, and money are saved and the application of this technology in chemical industry on a large-scale clearly underlines its practicability not only in academia but for everyone working in this field.

Z558419-1EA

CBILS©

A Revolutionary Tool for Ionic Liquid Synthesis

Roland St. Kalb and Michael J. Kotschan, proionic Production of Ionic Substances GmbH, Leoben, Austria; www.proionic.at; info@proionic.at

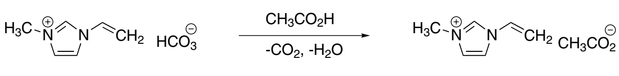
"When I first started to work with ionic liquids years ago, it always was an unfulfilled dream to investigate the most interesting ionic liquid structures in my field of research; either the substances were commercially not available in a suitable quality, were not even available at all, or there was no predictable synthetic route I trusted. It always took a long time to develop a new synthesis and to realize a new structure; the throughput of my screening was terrible," said Roland Kalb, organic chemist and scientific director of the Austrian company proionic Production of Ionic Substances GmbH. Michael Kotschan, managing director of proionic GmbH: "With CBILS© – **C**arbonate **B**ased **I**onic **L**iquid **S**ynthesis – we bring a revolutionary tool to the public, which stood the test of time perfectly in our own R&D for years. We are able to synthesize more than 20 brand new ionic liquids per person a day with ease, just using simple standard laboratory equipment."

How Does CBILS© Work?

Conventional ionic liquid synthesis is complicated, and often suffers from halogen impurities. In general, there was no systematic way to predicitably produce high-quality ionic liquids. CBILS© now offers the simplest synthetic method to Sigma-Aldrich customers.

For example, the synthesis of 1-vinyl-3-methylimidazolium acetate is performed by addition of one equivalent of acetic acid to the corresponding CBILS© precursor 1-vinyl-3-methylimidazolium hydrogencarbonate.

The anion is ultimately removed as carbon dioxide gas and exchanged by acetate. This type of reaction always works quantitatively with every Brønsted acid available, even very insoluble ones. The ionic liquid is isolated by simple evaporative removal of the solvent and the reaction by-product (water).



One Hundred Syntheses in One Week?

By using the CBILS© route for the synthesis of ionic liquids and analogous structures, it is possible for a single person, in one week's time, to synthesize 100 new substances via the combination of 10 precursors with 10 Brønsted acids. There is no need for the use of dry solvents, no halogen impurities or by-products are formed, no guesswork about the synthetic route, and no waste is generated. Just select the cation precursor and the anion (via the acid) of your choice, and make your dream ionic liquid a reality!

Details about CBILS© – Carbonate-Based Ionic Liquid Synthesis

Sigma-Aldrich now offers a selection of eleven CBILS© precursors for the synthesis of imidazolium, ammonium, phosphonium, pyrrolidinium, piperidinium, and morpholinium type ionic liquids in the form of their methylcarbonates and hydrogencarbonates. To synthesize your desired structure all you simply need to do is:

1. Choose the cation in the form of the corresponding CBILS© precursor.
2. Choose the anion in the form of the corresponding Brønsted acid.
3. Calculate the necessary stoichiometry to form the ionic liquid.
4. Mix the CBILS© precursor and the Brønsted acid and stir until CO_2 generation subsides – depending on the batch and the substance, this typically requires 5 minutes to 1 hour.

$$Z^+CH_3CO_3^- \xrightarrow{HA} Z^+A^- + CH_3OH + CO_2\uparrow$$

$$Z^+HCO_3^- \xrightarrow{HA} Z^+A^- + H_2O + CO_2\uparrow$$

5. Remove the solvent and reaction by-product (water or methanol) by rotary evaporation.

When performing your reaction, reserve extra head space in the reaction vessel (typically 2x the volume of the reaction mixture) to allow room for CO_2 foaming, especially for long-chained structures with detergent-like properties. Adding solvents such as ethanol or 2-propanol helps to prevent foaming. If you wish to avoid discoloration during the evaporation of the solvent, we recommend working under inert gas, otherwise weak discoloration is possible. Even so, discoloration does not generally affect the ionic liquids quality unless it is to be used in optical applications in the visible spectrum.

Now you can choose your anion out of thousands of commercially available Brønsted acids – from simple mineral acids to the most complicated, chiral and functionalized acids, from strong to weak ones, and from soluble to nearly insoluble ones. Because the chemical equilibrium is shifted continuously by the formation of gaseous carbon dioxide, the reaction always achieves a 100% conversion.

You can also use Brønsted acid precursors such as organic or inorganic anhydrides. For example, we successfully synthesized ionic liquid molybdates and tungstates using molybdenum oxide and tungsten oxide respectively, both of which are very insoluble in aqueous media. Although sluggish, both ionic liquids were formed at 100% conversion as evidenced by the slow, but continuous evolution of CO_2. Also the solubility, viscosity or aggregate state of the synthesized ionic liquid does not limit the reaction. Even water insoluble solids are formed perfectly and precipitate smoothly.

Stoichiometry

Calculating the exact reaction stoichiometry is critical, because the ionic liquid may be sensitive to unreacted free acid or carbonate precursor. The concentration of CBILS© precursors is indicated on the label and is lot specific. The concentration of the acid you are using must be known exactly via the certificate of analysis or alkalimetric titration. It should be known to within 1% accuracy.

By changing the stoichiometry of a diprotic Brønsted acid, you can synthesize hydrogenated anions with ease:

$$Z^+HCO_3^- + H_2A \longrightarrow Z^+HA^- + H_2O + CO_2\uparrow$$

$$2\,Z^+HCO_3^- + H_2A \longrightarrow Z^+_2A^{2-} + 2\,H_2O + 2\,CO_2\uparrow$$

Some anions are not accessible via Brønsted acids because the free acid is not stable or not known at all. An illustrative example is the thiocyanate anion SCN^-. Free thiocyanic acid (HSCN) is only stable at 0 °C in 5% aqueous solution and is not commercially available. In this case, you can use the corresponding ammonium salt, gently heating the reaction mixture to 60 °C for at least 30 minutes and removing the solvents at a temperature of at least 70 °C:

$$Z^+CH_3CO_3^- \xrightarrow{NH_4^+A^-} Z^+A^- + CH_3OH + CO_2\uparrow + NH_3\uparrow$$

$$Z^+HCO_3^- \xrightarrow{NH_4^+A^-} Z^+A^- + H_2O + CO_2\uparrow + NH_3\uparrow$$

Again, all reaction by-products are readily removed and the reaction reaches a 100% conversion. (**Caution!** Ammonia is harmful and corrosive. Work in an efficient fume hood.)

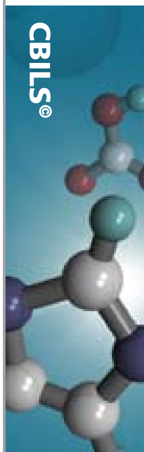
A second alternative to Brønsted acids is the reaction of a CBILS© carbonate precursor with a calcium, zinc, manganese or other metal salt, which results in the formation of an insoluble metal carbonate. For example, if you react calcium thiocyanate ($Ca(SCN)_2$) with a carbonate precursor, the desired thiocyanate-based ionic liquid is formed and calcium carbonate precipitates. The resultant solid can easily be removed by filtration or centrifugation.

Stability, Handling, and Storage

All CBILS© ionic liquid precursors are delivered in 40 to 60% aqueous or aqueous/methanolic solutions and are stable at room temperatures for years, unless stated otherwise (e.g. vinyl derivatives). The exact concentration is marked on the label and is lot specific. To maintain this concentration, the bottle should be closed immediately after use. Due to the methanol content, the solutions are weakly toxic. CBILS© ionic liquid precursors typically have pH values of 8 to 11 and are irritants, especially to the eyes.

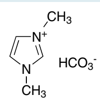
Other

Removal of the solvent to isolate the pure CBILS® ionic liquid precursors prior to the synthesis of an ionic liquid is not advised for any dialkylimidazolium hydrogencarbonate (1,3-dimethylimidazolium hydrogencarbonate, 1-ethyl-3-methylimidazolium hydrogencarbonate, 1-butyl-3-methylimidazolium hydrogencarbonate, 1-vinyl-3-methyl-imidazolium hydrogencarbonate) due to the irreversible formation of dialkylimidazolium carboxylates.



1,3-Dimethylimidazolium hydrogencarbonate, 50% solution in water — NEW

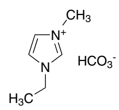
$C_6H_{10}N_2O_3$
FW: 158.18



670052-10G	10 g
670052-100G	100 g

1-Ethyl-3-methylimidazolium hydrogencarbonate, 50% solution in water — NEW

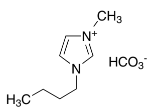
$C_7H_{12}N_2O_3$
FW: 172.18



670626-10G	10 g
670626-100G	100 g

1-Butyl-3-methylimidazolium hydrogencarbonate, 50% solution in water — NEW

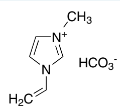
$C_9H_{16}N_2O_3$
FW: 200.23
[*366491-15-8*]



670723-10G	10 g
670723-100G	100 g

1-Vinyl-3-methylimidazolium hydrogencarbonate 50% solution in water — NEW

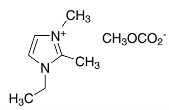
$C_7H_{10}N_2O_3$
FW: 170.17



670389-10G	10 g
670389-100G	100 g

1-Ethyl-2,3-dimethylimidazolium methylcarbonate, 50% solution in water/methanol (3:2) — NEW

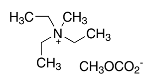
$C_9H_{16}N_2O_3$
FW: 200.23
[*625120-68-5*]



670952-10G	10 g
670952-100G	100 g

Triethylmethylammonium methylcarbonate, 50% solution in water/methanol (3:2) — NEW

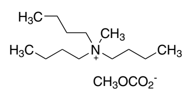
$C_9H_{21}NO_3$
FW: 191.27
[*113840-08-7*]



671053-10G	10 g
671053-100G	100 g

Tributylmethylammonium methylcarbonate, 50% solution in water/methanol (3:2) — NEW

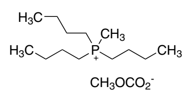
$C_{15}H_{33}NO_3$
FW: 275.49



671177-10G	10 g
671177-100G	100 g

Tributylmethylphosphonium methylcarbonate, 50% solution in water/methanol (3:2) — NEW

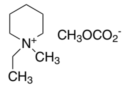
$C_{15}H_{33}PO_3$
FW: 292.45



671282-10G	10 g
671282-100G	100 g

1-Ethyl-1-methylpiperidinium methylcarbonate, 50% solution in water/methanol (3:2) NEW

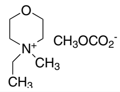
$C_{10}H_{21}NO_3$
FW: 203.28



671509-10G	10 g
671509-100G	100 g

4-Ethyl-4-methylmorpholinium methylcarbonate 50% solution in water/methanol (3:2) NEW

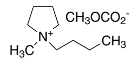
$C_9H_{19}NO_4$
FW: 205.25



671614-10G	10 g
671614-100G	100 g

1-Butyl-1-methylpyrrolidinium methylcarbonate 50% solution in water/methanol (3:2) NEW

$C_9H_{19}NO_3$
FW: 189.25



672386-10G	10 g
672386-100G	100 g

Dibutylphosphate and "Natural" Ionic Liquids

Roland St. Kalb and Michael J. Kotschan, proionic Production of Ionic Substances GmbH, Leoben, Austria; www.proionic.at; info@proionic.at

Ammonium and Phosphonium dibutylphosphates

Most commercially available ionic liquids are based on the prominent dialkyl- or trialkylimidazolium cations rather than on tetraalkylammonium or tetraalkylphosphonium cations. A major contributor to this fact may be the unusually high melting points and high viscosities of the latter ionic liquids. In contrast, short-chained quarternary ammonium and phosphonium dialkylphosphates, such as tributylmethylammonium, tributylmethylphosphonium, triethylmethylammonium or triethylmethylphosphonium dibutylphosphates, show the following typical properties:

- Acceptable viscosities: 1000–1500 mPas (20 °C), 200–300 mPas (40 °C), 20–30 mPas (90 °C)
- Freezing points: < –10 °C
- Good thermal stability, flash points between 150 °C and 250 °C
- No hydrolysis
- Stability towards strong bases (no acidic protons, in contrast to imidazolium type ionic liquids)
- Unusual solvent properties: a lack of aromatic π-electrons or free lone pairs of electrons on the cation results in less donor-acceptor interactions with solutes
- Miscible with water and polar solvents

The phosphonium dibutylphosphates show exceptional thermal stability. During thermal decomposition at 1300 °C, inorganic phosphates are formed that suppress the ignition of a flame. Therefore, these substances show excellent flame-retardant properties, and have already been tested for application as non-flammable hydraulic fluids.[1]

Treatment of tributylmethylphosphonium dibutylphosphate by a gas burner flame for 60 seconds.

Dialkylimidazolium dibutylphosphates

1-Ethyl-3-methylimidazolium dibutylphosphate (EMIM-DBP) and 1-butyl-3-methylimidazolium dibutylphosphate (BMIM-DBP) are two interesting alternatives to "everyday" EMIM and BMIM ionic liquids. They are free of halogen or sulfur impurities, stable to hydrolysis, and show low viscosities and melting points.

Chiral and "Natural" Ionic Liquids

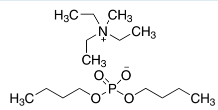
1-Ethyl-3-methylimidazolium L-(+)-lactate and 2-hydroxyethyltrimethylammonium L-(+)-lactate are two ionic liquids with chiral anions, which have the potential of chiral induction in enantioselective organic synthesis when used as solvents. The hydroxyl group in both the lactate anion and the 2-hydroxyethyltrimethylammonium cation possesses the ability to form hydrogen bonds to substrates and enzymes in biocatalytic reactions. Although chiral, they exhibit the typical properties of ionic liquids.

2-Hydroxyethyltrimethylammonium L-(+)-lactate and achiral 2-hydroxyethyltrimethylammonium acetate could be called "natural" ionic liquids due to the fact that they consist of common, naturally occurring ions. Thus, they are in our opinion among the "greenest" available ionic liquids since they are biodegradable, and apparently non toxic. 2-Hydroxyethyltrimethylammonium acetate has successfully been tested by proionic GmbH as a "green" medium in air-conditioning systems.

Reference: (1) Roland Kalb, 2006, "Basic Research and Development of non-flammable Hydraulic Safety Fluids"; http://www.bmvit.gv.at/innovation/verkehrstechnologie/isb/workshop/index.html

Triethylmethylammonium dibutylphosphate, purum NEW

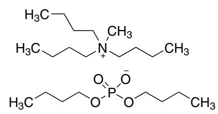
$C_{15}H_{36}NO_4P$
FW: 325.42



669849-5G	5 g
669849-50G	50 g

Tributylmethylammonium dibutylphosphate, purum NEW

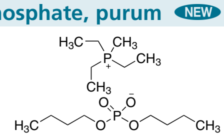
$C_{21}H_{48}NO_4P$
FW: 409.58



669962-5G	5 G
669962-50G	50 G

Triethylmethylphosphonium dibutylphosphate, purum NEW

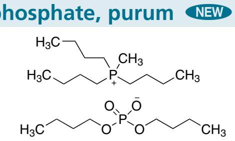
$C_{15}H_{36}O_4P_2$
FW: 342.39



670065-5G	5 g
670065-50G	50 g

Tributylmethylphosphonium dibutylphosphate, purum NEW

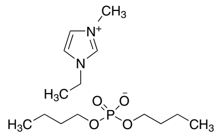
$C_{21}H_{48}O_4P_2$
FW: 426.55



670294-5G	5 g
670294-50G	50 g

1-Ethyl-3-methylimidazolium dibutylphosphate, purum NEW

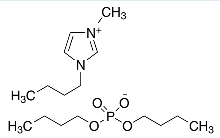
$C_{14}H_{29}N_2O_4P$
FW: 320.36



669636-5G	5 g
669636-50G	50 g

1-Butyl-3-methylimidazolium dibutylphosphate, purum NEW

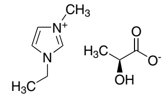
$C_{16}H_{33}N_2O_4P$
FW: 348.42



669733-5G	5 g
669733-50G	50 g

1-Ethyl-3-methylimidazolium L-(+)-lactate, purum NEW

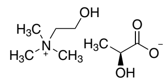
$C_9H_{16}N_2O_3$
FW: 200.23



669512-5G	5 g
669512-50G	50 g

2-Hydroxyethyltrimethylammonium L-(+)-lactate, purum NEW

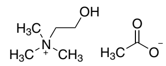
$C_8H_{19}NO_4$
FW: 193.24
[*888724-51-4*]



670391-5G	5 g
670391-50G	50 g

2-Hydroxyethyltrimethylammonium acetate, purum NEW

$C_7H_{17}NO_3$
FW: 163.21
[*14586-35-7*]



670189-5G	5 g
670189-50G	50 g

Trioctylmethylammonium thiosalicylate (TOMATS)

A novel, high-performance, task-specific ionic liquid for the extraction of heavy metals from aqueous solutions

Roland St. Kalb and Michael J. Kotschan, proionic Production of Ionic Substances GmbH, Leoben, Austria; www.proionic.at; info@proionic.at

Task-specific ionic liquids for the selective liquid/liquid extraction of heavy metals from aqueous systems were first published by Robin D. Rogers and co-workers in 2001.[1] Functionalized imidazolium cations with thioether-, urea- or thiourea-derivatized side chains act as metal ligating moieties, whereas the PF_6^- anion provides the desired water immiscibility (**Figure 1**). Nernst distribution ratios were reported for Cd^{2+} and Hg^{2+} to be $\leq$ 380.

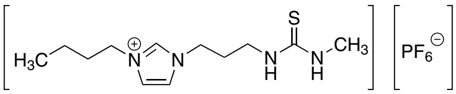


Figure 1: A thiourea derivatized ionic liquid

These ionic liquids were the first to contain specific functionalities to enable well defined chemical properties and may therefore be called "designer solvents."

However, these pioneering ionic liquids have some major drawbacks: the hexafluorophosphate anion is known to be quite unstable with respect to hydrolysis, producing toxic and corrosive HF or fluorides. The toxicity of the imidazolium cation is difficult to estimate and a toxicological study would be expensive. The disposal of these fluorous compounds is expensive and problematic. Additionally, the synthesis on a larger scale is complicated and the starting materials are expensive.

Trioctylmethylammonium thiosalicylate – a novel task-specific ionic liquid

To overcome these drawbacks – especially in consideration of possible industrial applications at larger scales – and to enhance the performance, proionic Production of Ionic Substances GmbH developed a new ionic liquid: trioctylmethylammonium thiosalicylate (TOMATS) (**Figure 2**).

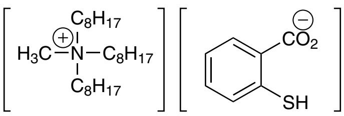


Figure 2: TOMATS

TOMATS contains no fluorine and is absolutely stable towards hydrolysis. Therefore, it does not release HF or fluorides, is non-corrosive, and is much easier to dispose. The low toxicity of the cation is known from related compounds like trioctylammonium chloride (a phase transfer catalyst) and thiosalicylic acid or its salts are typically classified as irritants. The distribution coefficients of heavy metals typically show values in the range of 50,000 to more than 2,000,000, which may be explained by the chelating effect of the ortho-positioned carboxylate group relative to the thiol functionality (which is well-known to form metal thiolate complexes). The synthesis is simple and can be done at industrial scales.

Application of TOMATS

Figure 3 shows the extraction of copper from a blue colored aqueous Cu^{2+}-tetramine phase. After addition of the TOMATS ionic liquid, and before shaking the test tube, diffusion zones can be seen (second test tube) showing a copper-free, colorless region and a dark copper-containing upper region. After shaking and separation of the phases, all the copper is extracted into the upper phase, as evidenced by the completely dark-colored ionic liquid layer (third test tube).

Figure 3: Extraction of Cu^{2+}

Phase separation sometimes takes quite a long time due to the high viscosity of TOMATS at 20 °C (1500 mPa·s). This drawback can be overcome by either adding a water-immiscible organic solvent like ethyl acetate, or by gentle heating of the mixture (to decrease the viscosity). Phase separation can be optimized by using a centrifuge or adding a small amount of sodium sulfate to the aqueous phase before shaking. If the aqueous phase still looks turbid, it can be filtered through a common membrane filter.

Characterization of TOMATS[3]

Appearance:	Olive green, viscous liquid
Relative Molecular Mass:	521.89 g/mol
Empirical Formula:	$C_{32}H_{59}NO_2S$
Solubility:	Soluble in alcohols, ethyl acetate, THF, acetonitrile, acetone, dichloromethane, DMSO; insoluble in water, hexane
Nernst Distribution Coefficients[4]:	Cd^{2+} >50,000; Cu^{2+} >50,000; Pb^{2+} and Hg^{2+} >100,000
Melting Point:	<30 °C
Refractive index:	n_D^{20} = 1.5185
Leaching into aqueous phase:	<100 ppm

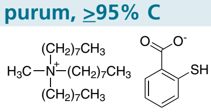
Viscosity and Density Temperature Dependence Data

	TOMATS 100%		TOMATS 95% (5% ethyl acetate)	
T [°C]	d (g/cm³)	η (mPa·s)	d (g/cm³)	η (mPa·s)
20	0.9556	1.500	0.9534	509
40	0.9445	352	0.9424	158
60	0.9325	119	0.9300	63
80	0.9213	50	0.9185	30

References: (1) Visser, A. E.; Swatloski, R. P.; Reichert, W. M.; Rogers, R. D.; Mayton, R.; Sheff, S.; Wierzbicki, A.; Davis, Jr., J. H. *Chem. Commun.* **2001**, 135. (2) *Decontamination of Heavy Metal polluted Process Water, Waste Water and Filter Cake with High Performance*, Roland St. Kalb, Regina Krachler, and Bernhard K. Keppler, EMChIE 2006 Conference Book, Vienna, May 3–5, 2006. (4) Aqueous phase with 5 to 50 ppm metal, 1:1 extraction, detection using AAS and ICP-AES.

Methyltrioctylammonium thiosalicylate purum, ≥95% C

$C_{32}H_{59}NO_2S$
FW: 521.88



08354-1G-F	1 g
08354-5G-F	5 g

Nitrile (Cyano) Functionalized Ionic Liquids

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Without a doubt, ionic liquids have captured the imagination of chemists as well as researchers in other scientific disciplines.[1] The principle application of ionic liquids in chemistry has been as alternative solvents for synthesis and catalysis. With this in mind, the search for ionic liquids with superior physical and chemical properties to those most frequently used has been met with considerable enthusiasm, especially with respect to task specific ionic liquids.[2] Of the numerous ionic liquids developed in this regard, a comparatively simple class of ionic liquid with alkyl-nitrile chains attached to the ionic liquid cation (see product list on page 15) have proven to be particularly useful, based on a series of impressive applications.

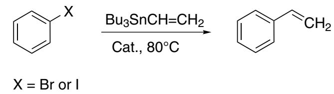
While the nitrile functionality is only weakly basic due to the presence of the ionic liquid cation (typically an imidazolium or pyridinium cation), it can nevertheless weakly coordinate to metal centers.[3] The net effect of such weak coordination is four-fold:

1. To facilitate the solubility of metal salts in the ionic liquids.
2. To be sufficiently labile so as not to suppress catalytic activity by blocking coordination sites during reaction.
3. To stabilize the catalyst, facilitate the formation of transition states, and therefore increase its lifetime.
4. To enhance the immobilization of the catalyst in the ionic liquid during product extraction, thereby improving recycling.

These advantages have been demonstrated to the greatest extent in palladium catalyzed C–C coupling reactions such as Suzuki, Heck, and Stille reactions.[4] **Figure 1** compares ionic liquid solutions following catalysis that illustrate the benefit of using the nitrile-functionalized system. Moreover, palladium nanoparticles separated after catalysis were analyzed by TEM and the images indicate that the nitrile-functionalized ionic liquid stabilizes palladium nanoparticles which are present as Pd(0) reservoirs. ICP analysis of the organic phase for palladium residues is often below the detection limit (1 ppm) suggesting that such ionic liquids could be useful in the synthesis of pharmaceuticals and liquid crystals where trace metal impurities must be extremely low.

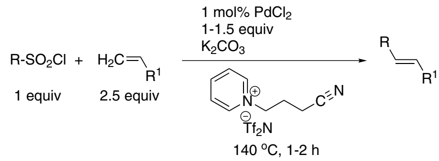
Figure 1: Comparison of ionic liquid-organic biphases after catalysis and TEM images of nanoparticles extracted from the ionic liquid phase; (left) [C_4py][Tf_2N] and (right) [C_3CNpy][Tf_2N]. Note the absence of precipitates and clarity of the organic phase with the nitrile-functionalized ionic liquid.

Nitrile-functionalized ionic liquids are considerably more effective for the immobilization of palladium catalysts for the transfer of a vinyl group in Stille reactions with respect to alkyl-substituted ionic liquids (**Scheme 1**).[5] Again, TEM analysis of nanoparticles extracted from the ionic liquids provide evidence for the stabilizing effect exerted by the nitrile pendant group on the metal center.



Scheme 1

While model substrates were used in the above examples, desulfitative Mizoroki-Heck-type arylation of alkenes using complex precursors can be performed efficiently in nitrile-functionalized ionic liquids (**Scheme 2**), again proving superior to the commonly used organic solvents and simple ionic liquids.[6]



Scheme 2

In a quite different application, ionic liquids are being used as non-volatile electrolytes in dye-sensitized solar cells, and those containing the nitrile functional group attached to imidazolium cations have been evaluated as electolytes in neat or binary systems (**Figure 2**).[7] Excellent energy conversion efficiencies were observed; ca. 8% in low light irradiations in the binary systems. Furthermore, excellent light soaking stability was observed during 1,000 hours of aging, indicating quite an extraordinary robustness.

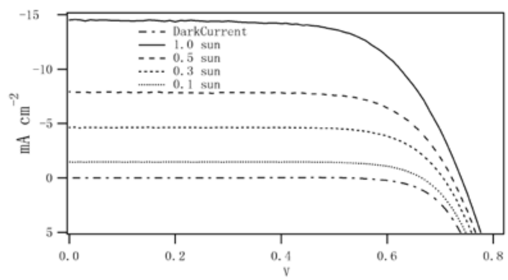


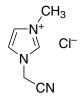
Figure 2: Current density-voltage characteristic of a DSC device containing a [C_3CNC_1im]-based ionic liquid electrolyte under AM 1.5 simulated full sunlight (100 mW cm^{-2}) illumination.

In general, these nitrile-derivatized ionic liquids can act as acetonitrile replacements wherever the advantage of having a non-volatile equivalent can be envisaged. If one searches the literature for reactions where optimum results are obtained in acetonitrile or other nitrile based solvents, then it is clear that these ionic versions offer considerable potential in synthesis and catalysis.

References: (1) For example see: (a) Seddon, K. R. J. *Chem. Technol. Biotechnol.* **1997**, *68*, 351. (b) Welton, T. *Chem. Rev.* **1999**, *99*, 2071. (c) Wasserscheid, P.; Keim, W. *Angew. Chem. Int., Ed. Engl.* **2000**, *39*, 3772. (d) Dupont, J.; Souza, R. F. D.; Suarez, P. A. Z. *Chem. Rev.* **2002**, *102*, 3667. (e) Chiappe C.; Pieraccini, D.; *J. Phys. Org. Chem.* **2005**, *18*, 275. (2) (a) Davis Jr., J. H. *Chem. Lett.* **2004**, *33*, 1072. (b) Fei, Z.; Geldbach, T. J.; Zhao, D.; Dyson, P. J. *Chem. Eur. J.* **2006**, *12*, 2122. (3) Zhao, D.; Fei, Z.; Scopelliti, R.; Dyson, P. J. *Inorg. Chem.* **2004**, *43*, 2197. (4) Zhao, D.; Fei, Z.; Geldbach, T. J.; Scopelliti, R.; Dyson, P. J. *J. Am. Chem. Soc.* **2004**, *126*, 15876. (5) Chiappe, C.; Pieraccini, D.; Zhao, D.; Fei, Z.; Dyson, P. J. *Adv. Synth. Catal.* **2006**, *348*, 68. (6) Reddy, D. S.; Zhao, D.; Fei, Z.; Rao Volla, C. M.; Dyson, P. J.; Vogel, P. *Synlett* **2006**, 3155. (7) Mazille, F.; Fei, Z.; Kuang, D.; Zhao, D.; Zakeeruddin, S. M.; Grätzel, M.; Dyson, P. J. *Inorg. Chem.* **2006**, *45*, 1585.

1-(Cyanomethyl)-3-methylimidazolium chloride purum NEW

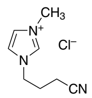
$C_6H_8ClN_3$
FW: 157.60
[*154312-63-7*]



04909-5G	5 g
04909-25G	25 g

1-(3-Cyanopropyl)-3-methylimidazolium chloride purum NEW

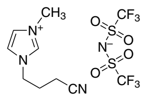
$C_8H_{12}ClN_3$
FW: 185.65
[*683224-96-6*]



04124-5G	5 g
04124-25G	25 g

1-(3-Cyanopropyl)-3-methylimidazoliumbis-(trifluormethylsulfonyl)imide NEW

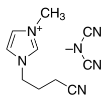
$C_{10}H_{12}N_4O_4S_2$
FW: 430.35
[*778593-18-3*]



38943-5G	5 g
38943-25G	25 g

1-(3-Cyanopropyl)-3-methylimidazolium dicyanamide, purum NEW

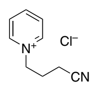
$C_{10}H_{12}N_6$
FW: 216.24



76902-5G	5 g
76902-25G	25 g

1-(3-Cyanopropyl)pyridinium chloride purum NEW

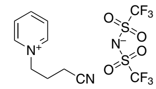
$C_9H_{11}ClN_2$
FW: 182.65



12136-5G	5 g
12136-25G	25 g

1-(3-Cyanopropyl)pyridinium bis(trifluoromethylsulfonyl)imide, purum NEW

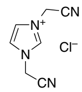
$C_{11}H_{11}F_6N_3O_4S_2$
FW: 427.34



16819-5G	5 g
16819-25G	25 g

1,3-Bis(cyanomethyl)imidazolium chloride, purum NEW

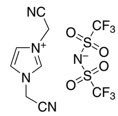
$C_7H_7ClN_4$
FW: 182.61



38904-5G	5 g
38904-25G	25 g

1,3-Bis(cyanomethyl)imidazolium bis(trifluoromethylsulfonyl)imide, purum NEW

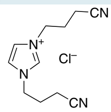
$C_9H_7F_6N_5O_4S_2$
FW: 427.30



28961-5G	5 g
28961-25G	25 g

1,3-Bis(3-cyanopropyl)imidazolium chloride, purum NEW

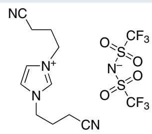
$C_{11}H_{15}ClN_4$
FW: 238.72



16959-5G	5 g
16959-25G	25 g

1,3-Bis(3-cyanopropyl)imidazolium bis(trifluoromethylsulfonyl)imide, purum NEW

$C_{13}H_{15}F_6N_5O_4S_2$
FW: 483.41



44493-5G	5 g
44493-25G	25 g

Nitrile (Cyano) Functionalized Ionic Liquids

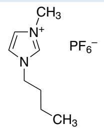
New Ionic Liquids for Catalysis

Several researchers have found that small impurities in ionic liquids exert a detrimental influence on the reaction outcome, particularly in catalysis. Dr. Annegret Stark of the Friedrich-Schiller University of Jena, Germany, has found that impurities such as water, unreacted amine (e.g. 1-methylimidazole), and traces of halides most frequently form during the preparation of ionic liquids. For example, she demonstrated the importance of the quality of ionic liquids employed in an olefin metathesis reaction (see *ChemFiles* Vol. 5, No. 6, p. 8).

Sigma-Aldrich is pleased to expand our portfolio of high-purity ionic liquids for catalysis. Typically, the water content is below 200 ppm and the excess halogen content is below 10 ppm.

1-Butyl-3-methylimidazolium hexafluorophosphate for catalysis

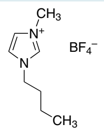
$C_8H_{15}F_6N_2P$
FW: 284.18
[*174501-64-5*]



18122-5G-F	5 g
18122-50G-F	50 g

1-Butyl-3-methylimidazolium tetrafluoroborate for catalysis

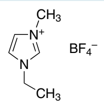
$C_8H_{15}BF_4N_2$
FW: 226.02
[*174501-65-6*]



39931-5G-F	5 g
39931-50G-F	50 g

1-Ethyl-3-methylimidazolium tetrafluoroborate for catalysis, ≥98.5% T

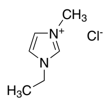
$C_6H_{11}BF_4N_2$
FW: 197.97
[*143314-16-3*]



39736-5ML-F	5 mL
39736-50ML-F	50 mL

1-Ethyl-3-methylimidazolium chloride, puriss., dry NEW

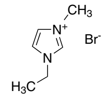
$C_6H_{11}ClN_2$
FW: 146.62
[*65039-09-0*]



53096-5G	5 g
53096-25G	25 g

1-Ethyl-3-methylimidazolium bromide puriss., dry NEW

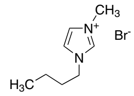
$C_6H_{11}BrN_2$
FW: 191.07
[*65039-08-9*]



03938-5G	5 g
03938-25G	25 g

1-Butyl-3-methylimidazolium bromide, puriss., dry, ≥98.5% HPLC NEW

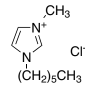
$C_8H_{11}BrN_2$
FW: 219.12
[*85100-77-2*]



64133-5G	5 g
64133-25G	25 g

1-Hexyl-3-methylimidazolium chloride, puriss., dry NEW

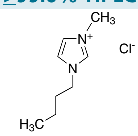
$C_{10}H_{19}ClN_2$
FW: 202.72
[*171058-17-6*]



15689-5G	5 g
15689-25G	25 g

1-Butyl-3-methylimidazolium chloride, dry, ≥99.0% HPLC

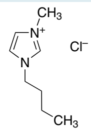
$C_8H_{15}ClN_2$
FW: 174.67
[*79917-90-1*]



55509-5G-F	5 g
55509-25G-F	25 g

1-Butyl-3-methylimidazolium chloride puriss., dry, ≥99.0% HPLC

$C_8H_{15}ClN_2$
FW: 174.67
[*79917-90-1*]

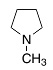


04129-5G-F	5 g
04129-50G-F	50 g

Ionic Liquid Precursors

N-Methylpyrrolidine, 97%

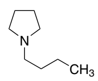
$C_5H_{11}N$
FW: 85.15
[*120-94-5*]



M79204-5ML	5 mL
M79204-100ML	100 mL
M79204-500ML	500 mL

1-Butylpyrrolidine, 98%

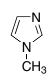
$C_8H_{17}N$
FW: 127.23
[*767-10-2*]



280372-250ML	250 mL

1-Methylimidazole, ≥99%, redistillation

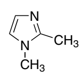
$C_4H_6N_2$
FW: 82.10
[*616-47-7*]



336092-100ML	100 mL
336092-1L	1 L
336092-2L	2 L

1,2-Dimethylimidazole, 98%

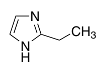
$C_5H_8N_2$
FW: 96.13
[*1739-84-0*]



136131-5G	5 g
136131-500G	500 g

2-Ethylimidazole, 98%

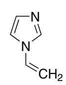
$C_5H_8N_2$
FW: 96.13
[*1072-62-4*]



239348-100G	100 g
239348-500G	500 g

1-Vinylimidazole, ≥99%

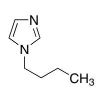
$C_5H_6N_2$
FW: 94.11
[*1072-63-5*]



235466-25G	25 g
235466-100G	100 g

1-Butylimidazole, 98%

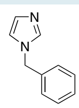
$C_7H_{12}N_2$
FW: 124.18
[*4316-42-1*]



348414-25G	25 g
348414-100G	100 g

1-Benzylimidazole, 99%

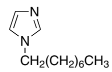
$C_{10}H_{10}N_2$
FW: 158.20
[*4238-71-5*]



116416-5G	5 g
116416-25G	25 g

1-Octylimidazole, purum, ≥98.0% GC

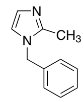
$C_{11}H_{20}N_2$
FW: 180.29
[*21252-69-7*]



75078-5ML	5 mL
75078-25ML	25 mL

1-Benzyl-2-methylimidazole, technical grade, 90%

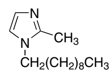
$C_{11}H_{12}N_2$
FW: 172.23
[*13750-62-4*]



369713-25ML	25 mL
369713-100ML	100 mL
369713-500ML	500 mL

1-Decyl-2-methylimidazole, 97%

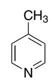
$C_{14}H_{26}N_2$
FW: 222.37
[*42032-30-4*]



433799-5ML	5 mL
433799-25ML	25 mL

4-Picoline, 99%

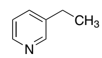
C_6H_7N
FW: 93.13
[*108-89-4*]



239615-50ML	50 mL

3-Ethylpyridine, 98%

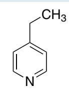
C_7H_9N
FW: 107.15
[*536-78-7*]



142395-5G	5 g

4-Ethylpyridine, 98%

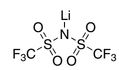
C_7H_9N
FW: 107.15
[*536-75-4*]



112437-25G	25 g
112437-100G	100 g

Bis(trifluoromethyl)sulfonimide lithium salt, ≥99.95%

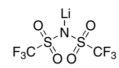
$C_2F_6LiNO_4S_2$
FW: 287.09
[*90076-65-6*]



544094-5G	5 g
544094-25G	25 g

Bis(trifluoromethyl)sulfonimide lithium salt, puriss., ≥99.0% ^{19}F-NMR

$C_2F_6LiNO_4S_2$
FW: 287.09
[*90076-65-6*]



15224-10G-F	10 g
15224-50G-F	50 g

Hydrophobic Ionic Liquids

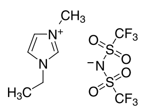
Ionic liquids, novel, salt-like materials with melting points below 100 °C, have gained much attention in recent years. This fascinating class of materials offers many benefits, including:

- **Negligible vapor pressure**
- **Tuneable solvent properties**
- **Nonflammability**
- **High ionic conductivity**
- **High thermal stability**

In collaboration with Covalent Associates, Inc., Sigma-Aldrich offers a set of extremely hydrophobic, thermally and hydrolytically stable ionic liquids.

1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, purum, ≥97.0% NMR

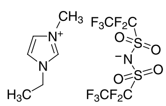
$C_8H_{11}F_6N_3O_4S_2$
FW 391.31
[*174899-82-2*]



11291-1G-F	1 g
11291-5G-F	5 g

1-Ethyl-3-methylimidazolium bis(pentafluoroethylsulfonyl)-imide, purum, ≥97.0% H-NMR

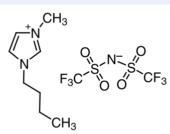
$C_{10}H_{11}F_{10}N_3O_4S_2$
FW 491.33
[*216299-76-2*]



39056-1G-F	1 g
39056-5G-F	5 g

1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, purum, ≥98.0% NMR

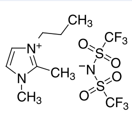
$C_{10}H_{15}F_6N_3O_4S_2$
FW 419.35
[*174899-83-3*]



77896-1G-F	1 g
77896-5G-F	5 g

1,2-Dimethyl-3-propylimidazolium bis(trifluoromethylsulfonyl)-imide, purum, ≥97.0% H-NMR

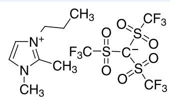
$C_{10}H_{15}F_6N_3O_4S_2$
FW 419.36
[*169051-76-7*]



50807-1G-F	1 g
50807-5G-F	5 g0

1,2-Dimethyl-3-propylimidazolium tris(trifluoromethylsulfonyl)-methide, purum, ≥97.0% HPLC

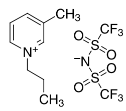
$C_{12}H_{15}F_9N_2O_6S_3$
FW 550.44
[*169051-77-8*]



74305-1G-F	1 g
74305-2.5G-F	2.5 g

3-Methyl-1-propylpyridinium bis(trifluoromethylsulfonyl)imide, purum, ≥97.0% HPLC

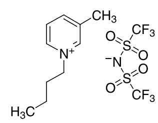
$C_{11}H_{14}F_6N_2O_4S_2$
FW 416.36
[*817575-06-7*]



30565-1G-F	1 g
30565-5G-F	5 g

1-Butyl-3-methylpyridinium bis(trifluoromethylsulfonyl)imide, purum, ≥97.0% H-NMR

$C_{12}H_{16}F_6N_2O_4S_2$
FW 430.39
[*344790-86-9*]



14654-1G-F	1 g
14654-5G-F	5 g

References

(1) Koch, V. R. et al. *J. Electrochem. Soc.* **1995**, *142*, L116.
(2) McEwen, A. B. et al. *J. Electrochem. Soc.* **1999**, *146*, 1687.
(3) Ngo, H. L. et al. *Thermochim. Acta* **2000**, *357–358*, 97.

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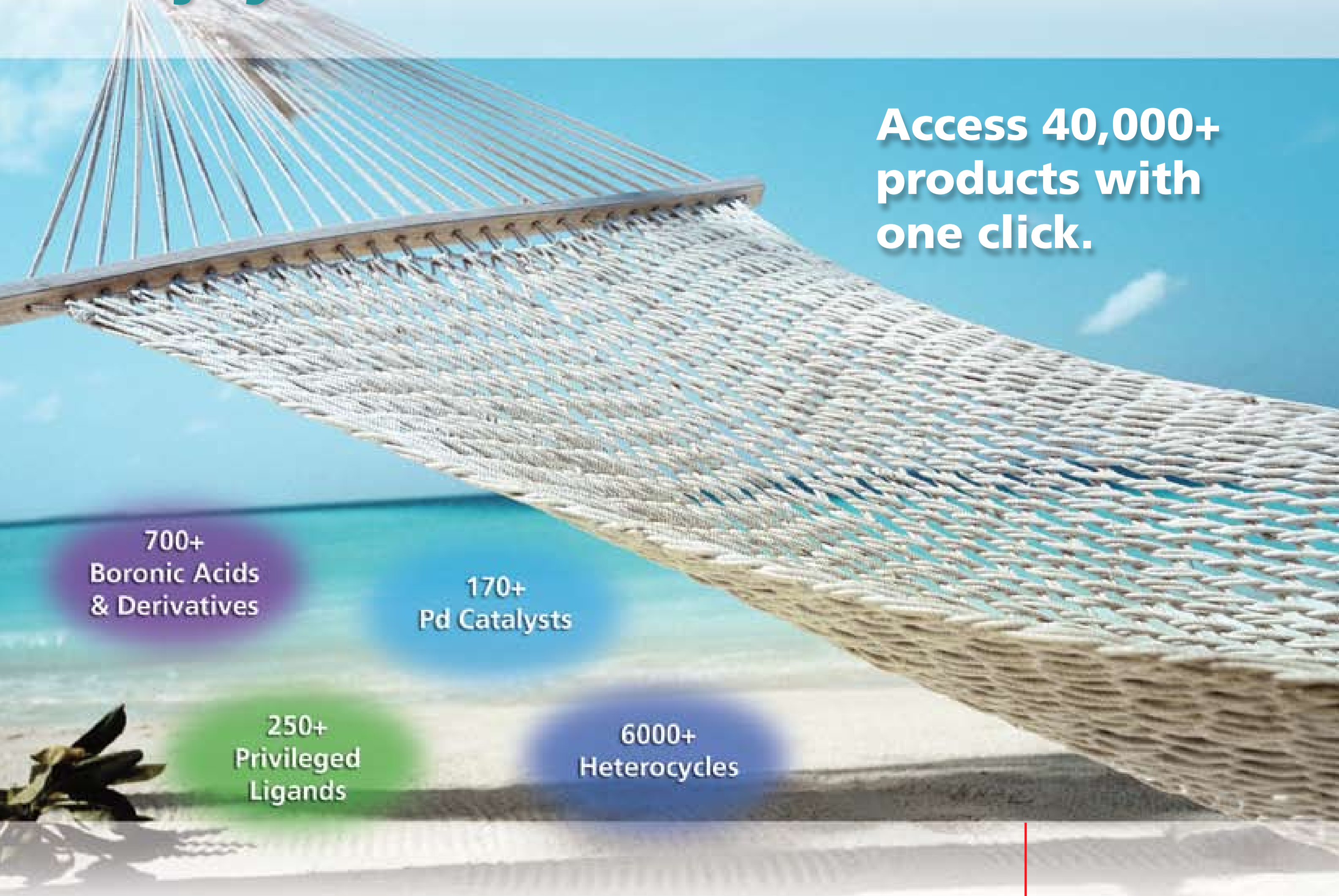

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