

# **Ionic Liquids Today**

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Thursday, 30<sup>th</sup> June, 2005.

Special Issue: 1st international congress on lonic Liquids, Salzburg, Austria COIL

June 19 – 22, 2005.

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#### I. Intro

By Thomas Schubert.

After a 4-days firework of very interesting talks from academia and as well from industry, in my opinion this  $1^{\rm st}$  congress on ionic liquids was an amazing success. The more than 400 (!) participants might indicate this, but also the interest from all leading companies, which supply ionic liquids, as (in alphabetical order except us) BASF, Degussa, Cytec, Merck, Scionix, Sigma-Aldrich, Solvent Innovation and of course from IOLITEC. On this occasion IOLITEC would like to thank the organising committee for this well organised congress with many excellent lectures and brilliant poster submissions.

The "Tabletop-Football" or "Tabletop-Soccer" at BASF's stall was beside the congress program probably the most remarkable feature: During the breaks the "BASIL-Arena" was highly frequented and hot matches were played. Unfortunately, this competition was a little bit to early for the young and inexperienced IOLITEC-team, which lost all games. We'll be ready at COIL 2 in Yokohama/Japan! Further insights were that



Peter Wasserscheid from the University of Erlangen does not only lead one of the best Ionic Liquids Research groups but also a well-trained Tabletop-Soccer team.



To us it's hard to evaluate all the impressions we took with us from COIL. Nevertheless, with this special issue, we try to formulate a brief, but, faithfully spoken, also subjective summary.



#### II. What we've learned at COIL

By Thomas Schubert & Tom Beyersdorff.

#### **Physical Data**

A lot of interesting talks were about physical data, e.g. conductivities, solubilities of gases in ionic liquids, viscosities and many more. We predict that simply on this topic an own congress could be possible or even necessary in the near future.

When we started with IOLITEC in 2003, our mission was to collect as many data as possible from substances known from literature or synthesized at our labs. In a couple of presentations, we cited Dr. Lowell King (taken from "Ionic Liquids in Synthesis" edited by Peter Wasserscheid and Tom Welton):

"If a new material is to be accepted as a technically useful material, the chemists must present reliable data on the chemical and physical properties needed by engineers to design processes and devices."

This statement demonstrates exactly what we think about ionic liquids and their chance of being used in applications, but it was extended at COIL by another very important conclusion by *Matthias Maase*, BASF AG:

#### "We do not sell purity, we sell performance"

he mentioned. The thought behind is obviously that if a material at a given purity shows the performance that was requested by the customer there's no need for a more expensive product with a higher purity.



Together with Seddon's consideration that impurities effect strong changes of physical parameters like viscosity or conductivity this idea consequently leads to the requirement of *physical data of completely characterized ionic liquids at a given purity*, with quantitative determination of impurities. Thus, from our point of view, a well-characterized material (purity & physical data!) will quickly gain reliance of potential users of ionic liquids.

A very systematic lecture about selected physicochemical properties of ionic liquids was presented by *Watanabe* (Yokohama National University). He correlated certain aspects of a given structure with electrochemical properties, e.g. a variety of cation at a fixed anion, with a physicochemical property, and vice versa.

On this occasion we would like to advert our two posters about determination of impurities by cyclovoltammetry (Metrohm PGSTAT 30) and by ion chromatography (cation and anion, Metrohm). We were very sorry that we just were able to offer a German version, since our colleague Andreas Bösmann just in the preparation phase suffered on a herniated disc. An English version will be published on our web-site soon.

In combination with our other in-house-analytics, such as

- residual water content by Karl-Fischer-Tritration (Metrohm 795, KFT Tirino)
- determination of conductivity (Metrohm 712)
- determination of viscosity (Brookefield)
- UV-VIS-Spectroscopy (Amersham)
- gas chromatography (Shimadzu)

and together with our strong academic network and our partner Metrohm, one of the world's leading specialists in ion analytics, we see ourselves in the position to solve the most analytical problems.

Finally, we do very appreciate the initiative from the NIST to build up a comprehensive Ionic Liquid database: <a href="http://www.iupac.org/projects/2003/2003-020-2-100.html">http://www.iupac.org/projects/2003/2003-020-2-100.html</a>



#### **Toxicity, Persistence and Sustainability**

The broad variety of already existing and of potentially designable ionic liquids will lead to the whole spectrum of properties of ionic liquids. Some of them are right now known to be toxic. The material that has the most hits in scientific publications, 1-butyl-3-methyl-imidazolium hexafluorophosphate is toxic and corrosive as well. But, and that's the good message, others are predicted to be even consumable! In addition, it has to be emphasized that ionic liquids are not inflammable below their decomposition temperature, which is often above 300°C, and that their negligible vapour pressure does not lead to an acute toxicity by inhalation. As a consequence, we are very unhappy with the identification of ionic liquids with *Green Solvents* in general.

Nevertheless, as Professor Jastorff (UFT, Bremen, Germany) mentioned, in terms of sustainability we have a real good chance for ionic liquids, to think holistic about technical performance, economic *and toxicity*. We felt very sad that he was not able to join COIL for his lecture to these topics. Prof. Brennecke filled the gap brilliantly and gave a very comprehensive overview about what is known about toxicity from ionic liquids today. A valuable information was the link to a database, where data to eco toxicity are collected:

Ecosar: Aquatic Toxicity and biodegradability

http://www.epa.gov/oppt/newchems/21ecosar.htm

**Episuite** 

http://www.epa.gov/opptintr/exposure/docs/episuite.htm

IOLITEC's point of view is that if a structural motif of an ionic liquid shows an outstanding performance at moderate production costs but with an unacceptable toxicological appearance, it should be possible to design and to tune the material with all the tools from synthetic organic and inorganic chemistry to be less toxic. In some cases, e.g. if the use of the ionic liquid saves significant amounts of energy, a moderate toxicity should be tolerated (but of course only if there's no less toxic material at comparable costs showing the same performance!).



#### A brief summary of interesting new applications

As already mentioned, we saw so many brilliant lectures and poster presentations that we're not in the position to report about all of them. This just should be interpreted as an incomplete and subjective abstract. IOLITEC tries to recognize all important influences from COIL at the earliest stage, to extend and to improve our services and products continuously.

#### a) Storage and delivery of hazardous gases

A very interesting application was presented by **D.J. Tempel** from **Air Products & Chemicals**: Ionic Liquids for the storage of hazardous gases. To dissolve and store aggressive gases like Phosphine or  $BF_3$  the used the corresponding ionic liquid based on a the tetrafluoroborate-anion. The actual status of commercialisation is prototype.

#### b) Neat Ionic Liquids as NMR-solvents

**Giernoth et al.** (University of Cologne) were able to use non-deuterated ionic liquids as solvents for the detection of Ethanol by using advanced NMR-techniques. This poster presentation received the 1<sup>st</sup> price at COIL's poster award. Congratulations!

# c) Electrolytes for Dye-Sensitized Solar-Cells (DSCs)

The development of dye-sensitized solar-cells, first introduced by *Grätzel* (ETH Lausanne) was accompanied from the development of ionic liquids nearly from the beginning: Ionic liquids seem to be the ideal electrolyte for this kind of application. DSCs have already reached prototypic status and are believed to be commercialised in the near future.

At COIL *Matsui* presented "Nanocomposite ion-gel electrolyte for dye – sensitized solar cells" in his lecture. *Wasserscheid et al.* (University of Erlangen) presented "Novel ionic liquids based electrolytes for dye-sensitized solar cells – characterization & assessment of quality" and



"Novel ionic liquids based electrolytes for dye-sensitized solar cells – synthetic strategies and ionic liquids cocktails" during the poster session. IOLITEC as the leading supplier for this kind of electrolytes offers any ionic liquid for their use in dye-sensitized solar cells. For example, we're in the position to offer 1-ethyl-3-methyl-imidazolium thiocyanate (EMIM SCN) in a guaranteed quality above 99.75% (water<500 ppm and bromide< 1000 ppm).

#### d) Solvents for the dimerization of olefins

**Olvier-Bourbigou** from the Institute Francaise Petrole (IFP) presented in her plenary lecture a couple of examples, where ionic liquids can be used as suitable solvents in catalysis. The dimerization of olefins has reached pilot plant status. In an impressive way, she demonstrated in which way the industrial plant could be simplified by using the ionic liquid-based process. If this application gets commercial, it will be a major breakthrough for ionic liquids in general!

#### e) Ionic Liquids for Head-Space-Chromatography

Another very interesting application in analytics is the use of ionic liquids as solvents in headspace chromatography. Since they have a negligible vapour-pressure, they seem to be ideal solvents for this application. **Andre et al.** described three examples where ionic liquids were used successfully with good results in this context.

#### f) Ionic Liquids as electrolytes for the deposition of metals

An electrochemically stable, non aqueous and non vaporizable electrolyte seemed to be just a dream for the deposition of metals, especially for those, which can not be deposited from aqueous media such as Al, Mg, Ti and many others. With Ionic Liquids this dream is close to be come true: *Hempelmann* (University of Saarland) demonstrated that e.g. Al can be deposited in a nanostructured quality on other metals.

# IoLiTec

# **Ionic Liquids Today, COIL Special-Issue**

Please note that IOLITEC's division R&D-services offers contract R&D to design special, customized solutions (deposition of metals & alloys) and sells as well state-of-the-art-electrolytes at fair prices!

#### g) Task-Specific Ionic Liquids (TSILs)

Many lectures and poster presentations attended to the topic "Task-Specific-Ionic-Liquids" (TSILs). TSILs are functionalised Ionic Liquids designed for "specific tasks", e.g. selective extraction of metal ions or as tag for solid-phase-chemistry.

#### h) Ionic Liquids as solvents for a novel type of reactor

**Vaultier et al.** used the conductivity of ionic liquids to design a new kind of reactor which is able to mix two or more droplets just by changing/moving the electrical field. This technology is very interesting for it's use in any kind of automated synthesis.

# III. Special offers

By Tom Beyersdorff

1-Ethyl-3-methyl-imidazolium thiocyanate: EMIM SCN

S=C=N<sup>-</sup>

EMIM SCN is probably the most often used electrolyte in Dye-Sensitized-Solar-Cells (DSCs) with low viscosity and high conductivity. We now offer this material in two grades of purity (99% and 99+%).



# My special offer\*:

<b>EMIM SCN (99%)</b>	IL-007-25g	90,00€
	IL-007-50g	170,00€
	IL-007-100g	330,00€
	IL-007-250g	750,00€
EMIM SCN (99+%)	IL-007+-25g	100,00€
	IL-007+-50g	190,00€
	IL-007+-100g	360,00€
	IL-007+-250g	850,00€

# 1-Allyl-3-methyl-imidazolium chloride: AllylMIM Cl

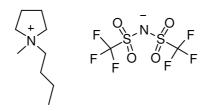
This material is know to dissolve up to 15% of cellulose at 60°C and will probably also dissolve many other polysaccharides.

# My special offer\*:

AllyIMIM CI (98%)	IL-022-25 g	70,00€
	IL-022-50 g	130,00€
	IL-022-100 g	190,00€
	IL-022-250 g	425,00€



# *N*-Butyl-*N*-methyl-pyrrolidinium bis(trifluoromethylsulfonyl)imide: BMPyrr NTf<sub>2</sub>



The perfect material for electrochemistry: large ECW, high thermal stability and highly hydrophobic.

This ionic Liquid is now also available in two grades of purity (99% and 99+%).

# My special offer\*:

BMPyrr NTf <sub>2</sub> (99	%)	IL-035-25g	60,00€
		IL-035-50g	100,00€
		IL-035-100g	185,00€
		IL-035-250g	420,00€
BMPyrr NTf <sub>2</sub> (99+%)		IL-035+-25g	70,00 €
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<i>IL-035+-50g</i>	110,00€		
		IL-035+-100g	200,00€
		IL-035+-250g	470,00 €

<sup>\*</sup> All special offers are valid from Juli 15<sup>th</sup> until August 31<sup>st</sup>.

Prices for larger amounts and bulk-quantities on request.



#### **Impressum**

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