FRONTIERS IN CHEMISTRY

LEADING FROM CHANGING FACES OF HUMAN BEINGS OR LOCATION OR ORGANIZATION.

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PREFACE

The Children's Club science programme has always been a challenge to us. In the past we have been conducting this programme for a number of years without any break. Every time, by a conscious effort, a theme has been chosen and all the presentations have been revolving around the theme chosen. This year "**Frontiers in Chemistry**" has been chosen as the theme, since it is felt that Chemistry is changing its face to a great extent due to its overlap on side with mathematics and physics and on the other side with biology. This overlap on both extremes has resulted chemistry to loose its original colour and it now exhibits a variety of colours like a rainbow.

The chemical processes have to change its inventory to bio sources and the chemical industry may turn out to be a biochemical based in the coming decade. We have already started hearing about bio refinery, bio-diesel and probably it will also lead to biochemical based chemical industry soon. There can be so many reasons for this change over.

On the scientific side, the introduction of new techniques which can virtually **see** at molecular level has revolutionized the way chemistry is practiced today. One has started looking at nano scale and started designing and fabricating tools at nano scale. This can have far reaching consequences and the expected surprises can be in almost all sectors of human endeavour.

It is therefore natural that the teaching and learning of Chemistry have also to change. This is evident from the methodology that one has to adopt since lecture based courses are not longer appealing and one has to use a variety of soft ware tools to demonstrate and make the molecules **perform** so that the teacher and the taught is enjoying the knowledge transfer process in a totally different platform.

Keeping all these factors into account, this years chemistry programme has been designed around the **Frontiers of Chemistry**. The lectures will be delivered by the research fellows of the National Centre for Catalysis Research, IIT Madras. We express our sincere thanks to each one of them for their effort.

The Science programme of the Children's club has been originally conceived by Mr.Narayanaswamy, the Secretary of the club. His support and enthusiasm have been the sole driving force for conducting this programme year after year. If there is any good arising out of this programme, the credit should naturally go to him.

We do hope you will enjoy the presentations and also find them enough challenging for your scientific curiosity.

Chennai:600036 B.Viswanathan

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CHAPTER 1
INTRODUCTION TO FRONTIERS IN CHEMISTRY

B. Viswanathan

1. Introduction

The study of chemistry is changing its face. In 20th century, the study of chemistry required some foundations in mathematics. But as the 21st century is unfolding, the emphasis in chemistry is shifted to biology. In fact, the demarcation line that existed between chemistry and biology is slowly vanishing and now one either talks of chemical biology or biological chemistry. This change over is going to have many ramifications in the study of chemistry. This shift in emphasis will have many other consequences. Some of the changes that one can expect in the study of chemistry would be that the study of atoms and molecules and clusters will become routine and mapping of the wave functions will become possible and hence the chemical reactivity will become a predictable parameter.

The consequence of the overlap of chemistry will biology will manifest remarkably in our study of the energy conversion processes. Hitherto the energy conversion processes are governed by the Carnot limitation since the known and practiced energy conversion processes always involved thermal conversion in one step or other. As all of us know that thermal route for energy conversion is the least efficient one. Living systems as well as the individual components of living systems function with internal generation of energy. Internal generation of energy probably accounts for high efficiency. Chemists have to formulate energy conversion devices as efficient as the living systems and probably this will be one way of understanding life.

The chemical industry has been toying with the idea of achieving 100% selectivity and the possibility of by-product formation has been one of the stumbling blocks for this goal. This has resulted in desire for 100% atom economy and hence led to the concept of green chemistry. We will revert back to this concept at a later stage. Chemical industries have to change their raw material inventory and hence the process principles also have to be changed considerably.

Synthetic chemistry is the corner stone of chemical industry. Synthetic methodologies have to be changed alternate media, (ionic liquids) reaction conditions (high T and P) have to be room temperature and atm pressure. This means that the basic governing principles have be modulated and reformulated.

2. The sub-disciplines where remarkable changes are expected:

Let us consider some of the changes that can be expected. This aspect has been considered in the following paragraphs some selected title-wise the challenges one will face in the changing scene.

2.1. Synthesis **and Manufacturing:** This will involve creating and exploiting New Substances and New Transformations. Some Challenges for Chemists and Chemical Technologists can be listed as follows:

(i) Develop methods that will enable synthesis of all important molecules in reasonable yields using compact synthetic schemes, so that no useful compound is inaccessible to practical synthesis.
(ii) Develop novel transformations that perform with the selectivities typical of enzymatic reactions, so that geometric factors are more important than the intrinsic reactivity of a molecule.
(iii) Use computer methods to design important target molecules and design efficient ways to make them.
(iv) Exploit combinatorial methods to discover important properties in synthetic materials.
(v) Design synthetic procedures that can be varied systematically for the purpose of optimizing specific properties of the reaction products.
(vi) Understand fully the basic chemical and physical properties of surfaces, especially those of solid catalysts.
(vii) Develop versatile and reliable synthetic methodologies for hard matter (micro-structured materials such as nanoparticles and porous solids) that are as effective as those for synthesis of soft matter (complex organic and bio-molecules).

2.2. Chemical and Physical Transformations of Matter:

This practice of chemistry will give rise to some challenges to the chemists. They can be listed as follows:

(i) They have to perfect the tools to study reaction mechanisms of chemical and biochemical reactions, so the processes can be observed directly and more efficient syntheses can be designed rationally.
(ii) They have to develop reliable computer methods to predict the detailed pathways and rates of unknown chemical reactions, avoiding the need for creating and measuring them to determine their practicality.
(iii) They need to understand the chemistry and properties of large molecules, including biopolymers, to the level that small-molecule chemistry is understood.
(iv) They have to understand the behavior of molecules and substances in unusual environments: at extreme temperatures or pressures, absorbed on solid surfaces, or under shear flow.
(v) They have to learn the chemistry of molecules and substances in their excited states, or at or near their critical points, and at the nanoscale level in which surface characteristics can dominate bulk properties.

2.3. Isolating, Identifying, Imaging, and Measuring Substances and Structures

(i) The tools have to be improved for imaging and determining structure so that detailed chemical structures can be determined with tiny amounts of non-crystalline material.
(ii) The ability of instruments to detect and quantify very low concentrations of important substances, even in very small volumes has to be achieved.
(iii) Effective methods for detecting dangerous materials, even when they are hidden have to be formulated.
(iv) Understand the chemistry that occurs in interplanetary and interstellar space, for which spectroscopy is the primary tool available.
(v) Develop instruments for on-line process control that bring the power of modern analytical and structure-determination methods to chemical manufacturing technology

2.4. **Chemical Theory and Computer Modeling**: From Computational Chemistry to Process Systems Engineering

(i) Develop computer methods that will accurately predict the properties of unknown compounds.
(ii) Develop reliable computer methods to calculate the detailed pathways by which reactions occur in both ground states and excited states, taking full account of molecular dynamics as well as quantum and statistical mechanics.
(iii) Develop reliable force fields for molecular mechanics calculations on complex systems, including those with metallic elements.
(iv) Invent computer methods to predict the three-dimensional folded structure of a protein—and the pathway by which folding occurs—from its amino acid sequence, so information from the human genome can be translated into the encoded protein structures.
(v) Devise experimental tests to establish the reliability of new theoretical treatments.

2.5 The Interface with Biology and Medicine

(i) Understand fully the chemistry of life, including the chemistry of the brain and memory.
(ii) Invent and learn to manufacture effective antiviral agents and antibiotics to fight all serious diseases, including those caused by drug-resistant pathogens.
(iii) Invent medicines that go beyond treatment to provide cure or prevention of life-limiting conditions and diseases such as cancer, Alzheimer’s disease, mental illness, and diabetes.
(iv) Invent better ways to deliver drugs to their targets, including devices that can function as artificial organs.
(v) Learn how genetic variation among individuals will affect their responses to particular medicines.
(vi) Invent biocompatible materials for organ replacements and for artificial bones and teeth.

2.6. Materials by Design

(i) Invent improved structural materials that are stable at high temperatures and easily machined.
(ii) Invent materials with useful electrical and optical properties, including high-temperature superconductivity.
(iii) Invent materials that are lighter, stronger, and more easily recycled.
(iv) Invent materials for surface protection (paints and coatings) that are truly long-lasting and rugged.
(v) Understand and utilize the properties of nanoscale materials and materials that are not homogeneous.
(vi) Build materials with the kind of actuating response found in physiological systems such as muscle.
(vii) Develop and process materials in which complex structural assembly occurs spontaneously or with minimal guidance and in useful timescales to produce durable systems with diverse utility.
(viii) Create nanomaterials technology from nanoscale chemical science.

2.7. Atmospheric and Environmental Chemistry:

(i) Elucidate the entire complex interactive chemistry of our biosphere— the atmosphere, the earth, and its lakes, rivers, and oceans—and provide the scientific basis for policies that preserve our environment
(ii) (ii) Ensure that chemical manufacturing and chemical products are environmentally and biologically benign, never harmful.
(iii) (iii)Learn how to make products that are stable over their necessary life but then undergo degradation so they do not persist in the environment or in living creatures
(iv) Invent agricultural chemicals that do not harm unintended targets in any way and are not overly persistent.
(v) Develop selective catalysts that enable the manufacture of useful products without producing unwanted waste products and without using excessive energy
(vi) Invent processes for the generation and distribution of energy that do not release greenhouse gases or toxic contaminants into the atmosphere.
(vii) Help humans control their population growth by inventing birth control methods that are safe and effective, inexpensive, and widely available and accepted.

2.8. Energy: Providing for the Future:

(i) Develop more stable and less expensive materials and methods for the capture of solar energy and its conversion to energy or to useful products.
(ii) Design inexpensive, high-energy-density, and quickly rechargeable storage batteries that make electric vehicles truly practical.

(iii) Develop practical, less expensive, more stable fuel cells with improved membranes, catalysts, electrodes, and electrolytes.
(iv) Develop materials, processes, and infrastructure for hydrogen generation, distribution, storage, and delivery of energy for vehicles.
(v) Develop photo-catalytic systems with efficiencies great enough to use for chemical processing on a significant scale.
(vi) Learn how to concentrate and securely deal with the radioactive waste products from nuclear energy plants.
(vii) Develop practical superconducting materials for energy distribution over long distances.

The eight subdivisions are in no way exhaustive but they have been chosen because of familiarity and directions in these topics can be formulated with certain degree of certainty.

3. Green Chemistry:

Green chemistry is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of chemical products." The generally accepted principles of Green Chemistry are:

1. It is better to prevent waste than to treat or clean up waste after it is formed.
2. Synthetic methods should be designed to maximize the incorporation of all materials used in the process to the final product
3. Whenever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.
4. Chemical methods should be designed to preserve efficacy of function while reducing toxicity.
5. The use of auxiliary substances (e.g. solvents, separation agents, etc.) should be made unnecessary whenever possible and, innocuous when used.
6. Energy requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure.
7. A raw material or feedstock should be renewable rather than depleting wherever technically and economically practicable.
8. Unnecessary derivatization (blocking group, protection/deprotection, and temporary modification of physical/chemical processes) should be avoided whenever possible.
9. Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.
10. Chemical products should be designed so that at the end of their function they do not persist in the environment and break down into innocuous degradation products.
11. Analytical methods needed to be further developed to allow for real time, in process monitoring and control prior to the formation of hazardous substances.
12. Substances and the form of a substance used in a chemical process should be chosen so as to minimize the potential for chemical accidents, including releases, explosions, and fires.

3.1. Is Green Chemistry an Ethical Imperative for Research in Chemistry?

To answer this question we must consider the following points:

Do we live in a sustainable civilization?

Is the pursuit of sustainability an ethical imperative for humanity?

What role can chemistry play in allowing a high technology civilization to become sustainable?

Is moving technology towards sustainable processes an ethical imperative for chemists?

This leads us to the question of sustainability

3.2. Sustainability: An Ethical Imperative?

In a brilliant book, which should be read by anyone concerned about sustainability, "The Imperative of Responsibility: In Search of Ethics for the Technological Age" (The University of Chicago Press, Chicago, 1984) Hans Jonas argues that there is a need for a new ethics that will better enable our civilization to deal with the power over the ecosphere that it has acquired through science and technology.

The book opens as follows:

"All previous ethics — whether in the form of issuing direct enjoinders to do and not to do certain things, or in the form of defining principles for such enjoinders, or in the form of establishing the ground of obligation for obeying such principles — had these interconnected tacit premises in common: that the human condition, determined by the nature of man and the nature of things, was given once for all; that the human good on that basis was readily determinable; and that the range of human action and therefore responsibility was narrowly circumscribed. It will be the burden of the present argument to show that these premises no longer hold, and to reflect on the meaning of this fact for our moral condition. More specifically, it will be my contention that with certain developments of our powers the *nature of human action* has changed, and, since ethics is concerned with action, it should follow that the changed nature of human action calls for a change in ethics as well: this not merely in the sense that new objects of action have added to the case material on which received rules of conduct are to be applied, but in the more radical sense that the qualitatively novel nature of certain of our actions has opened up a whole new dimension of ethical relevance for which there is no precedent in the standards and canons of traditional ethics."

The greatly increasing pressure of technology-based human activity on the ecosphere has given rise to the uncertainty and the insecurity captured in the concept of sustainability.

Can we continue to operate our civilization as we have been doing without spoiling or even ruining the future possibly for ourselves and almost certainly for our descendants?

Since much of the technological power underlying the sustainability dilemma has been devised by chemists, it is reasonable for chemists to ask how chemistry might be advanced to contribute to the sustainability of our civilization.

Green chemistry is arising as a field representing the practical expression of the willingness of chemists to turn technology towards sustainability.

4. The imperatives of Nano-technology:

Nanotechnology is an enabling technology that will impact electronics and computing, materials and manufacturing, energy, transportation and so on.

- The field is interdisciplinary but everything starts with material science. Challenges include:
    - Novel synthesis techniques
    - Characterization of nanoscale properties
    - Large scale production of materials
    - Application development

- Opportunities and rewards are great and hence, tremendous worldwide interest

- Integration of this emerging field into engineering and science curriculum is important to prepare the future generation of scientists and engineers

5. Dreaming in chemistry

Chemists are familiar with dreaming. This dreaming exercise is going to continue and list us list one of the sets of dream reactions for which heterogeneous catalysts have to be formulated. A few of the reactions are given below

$CH_4 + ½ O_2 \rightarrow CH_3OH$

$CH_4 + 1/2O_2 \rightarrow CO + 2H_2$

$2CH_4 + O_2 \rightarrow C_2H_4 + 2H_2O$

$nCH_4 \rightarrow C_nH_{2n+2} + (2n-2)H_2$

$DME \rightarrow C_2H_5OH$

$H_2 + O_2 \rightarrow H_2O_2$

$2NO \rightarrow N_2 + O_2$

$2N_2 + 2H_2O + 5O_2 \rightarrow 4HNO_3$

Other processes which will dominate the scene include the following:

- Heterogeneous catalysts for assymmetric synthesis
- Photolytic water splitting (hydrogen economy)
- Biomimetics, synthetic enzymes
- Non-thermal processes in general

In addition to this heterogeneous catalysis, it is possible that the sensors field also will face considerable changes. This is because that we have learnt how to functionalize the surfaces and hook bio-molecules on the surfaces which will remarkably change our capability for detection and quantification. It is clear that chemists are in for a tremendous change in the next few years. In Table 1 what are new in chemistry are listed. It must be stated that this is only an indicative list and no way an exhaustive list.

Table 1 What is new in Chemistry

• **Atmospheric chemistry** • **Biotechnology** • **Cell biology** • **Cell and molecular biology** • **ceramics Composites** • **Computational Chemistry** • **Crystallography** • **Electrochemistry** • **Harmonic analysis** • **Liquid crystals** • **Magnetic technology** • **Marine geology and geo-physics** • **Materials science** • **Microbiology** • **Microscopy** • **Molecular biology**	• **Nanotechnology** • **Oceanic sciences** • **Optics and photonics** • **Organic chemistry** • **Particle technology** • **Petroleum and geo-systems Photonic band gap materials** • **Photonics** • **Polymers and plastics** • **Process industries** • **quantum computation** • **Quantum optics and atom optics** • **Radiocarbon** • **Soil science** • **Surface science** • **Thermodynamics** • **Tri-biology** • **The ultra-fast phenomena**

CHAPTER 7
IONIC LIQUIDS

C. M. Janet

I. Introduction

An ionic liquid (IL) is a recently emerged new class of solvents which often exist as fluid at room temperature. They consist entirely of ionic species. In a broad sense, the term includes all molten salts, for instance, sodium chloride at temperatures higher than 800 °C. Today, however, the term "ionic liquid" is commonly used for salts whose melting point is relatively low (below 100 °C). In particular, the salts that are liquid at room temperature are called room-temperature ionic liquids or RTILs. They have many fascinating properties which make them of fundamental interest to all chemists, since both the thermodynamics and the kinetics of reactions carried out in ionic liquids are different to those that take place in conventional molecular solvents and also the chemistry is different and unpredictable at our current state of knowledge.

Designing of IL can be done by varying two components, they are anions and cations. Either the solvents can be designed with a particular end use in mind or to possess a particular set of properties. Hence the term designer solvents have been assigned to the ionic liquids.

The first room-temperature ionic liquid $[EtNH_3][NO_3]$ (m.pt. 12 °C) was discovered in 1914 , but interest did not develop until the discovery of binary ionic liquids made from mixtures of aluminum (III) chloride and *N*-alkylpyridinium or 1, 3 dialkylimidazolium chloride. In general, ionic liquids consist of a salt where one or both the ions are large, and the cation has a low degree of symmetry. These factors tend to reduce the lattice energy of the crystalline form of the salt and hence the melting point will be lower. Ionic liquids come in two main categories, namely simple salts (made of a single anion and cation) and binary ionic liquids (salts where equilibrium is involved). For example, $[EtNH_3][NO_3]$ is a simple salt whereas mixtures of aluminum (III) chloride and 1,3-dialkylimidazolium chlorides (a binary ionic liquid system) contain several different ionic species.

Being advantageous over conventional organic solvents, ILs have attractive physicochemical properties such as negligible vapor pressure even at elevated temperatures, excellent thermal and chemical stability, high ionic conductivity up to 0.1 S cm^{-1}, high mobility, high heat capacity, cohesive energy density, low toxicity and non-flammability. Furthermore, as the physicochemical properties of ILs strongly depend on the species of cation and anion and the length of the lateral alkyl groups on the heterocyclic rings, alternation of the anion or the length of the alkyl groups allows fine tuning of the physico chemical properties such as viscosity, solvation, catalytic activity, hydrophobicity, density and melting points. For example, the melting points of ionic liquids are a function of the alkyl chain length and depending upon the chain length it can form liquid crystalline phases. Another important property that changes with structure is the miscibility of water in these ionic liquids. This behavior can be of substantial benefit when carrying out solvent extractions or product separations, as the relative solubilities of the ionic and extraction phase can be adjusted to make the separation as easy as possible. Cations are normally big bulky and asymmetric accounting for the low melting points. The anion contributes more to the overall characteristics of the IL and determines the air and water stability.

Many classes of chemical reactions, such as Diels-Alder reactions and Friedel-Crafts reactions, can be performed using ionic liquids as solvents. Recent work has shown that ionic liquids can serve as solvents for bio-catalysis. The miscibility of ionic liquids with water or organic solvents varies with side chain lengths on the cation and with choice of anion. They can be functionalized to act as acids, bases or ligands and have been used as precursor salts in the preparation of stable carbenes. Because of their distinctive properties, ionic liquids are attracting increasing attention in many fields, including organic chemistry, electrochemistry, catalysis, physical chemistry, and engineering for instance magnetic ionic liquid.

IL are environmentally friendly alternatives to organic solvents for liquid-liquid extractions, catalysis, separations and electrochemistry. IL will reduce or eliminate the related costs, disposals requirements, and hazards associated with volatile organic compounds. The ability to fine tune the properties of the IL medium will allow replacing the specific solvents in a variety of different processes.

Room temperature ionic liquids

We are also always on the look out for new potentially environmentally benign separation media. One such possibility is the class of solvents known as room temperature ionic liquids. Room temperature ionic liquids consist of bulky and asymmetric organic cations such as 1-alkyl-3-methylimidazolium, 1-alkylpyridinium, N-methyl-N-alkylpyrrolidinium and ammonium ions. A wide range of anions is employed, from simple halides, which generally inflect high melting points, to inorganic anions such as tetrafluoroborate and hexafluorophosphate and to large organic anions like bis-trifluorsulfonimide, triflate or tosylate. There are also many interesting examples of uses of ionic liquids with simple non-halogenated organic anions such as formate, alkylsulfate, alkylphosphate or glycolate. As an example, the melting point of 1-butyl-3-methylimidazolium tetrafluoroborate or **[bmim] $[BF_4]$** with an imidazole skeleton is about -80 °C, and it is a colorless liquid with high viscosity at room temperature.

It has been pointed out that in many synthetic processes using transition metal catalyst; metal nanoparticles play an important role as the actual catalyst or as a catalyst reservoir. It also been shown that ionic liquids (ILs) are an appealing medium for the formation and stabilization of catalytically active transition metal nanoparticles. More importantly, ILs can be made that incorporate co-ordinating groups, for example, with nitrile groups on either the cation or anion (CN-IL). In various C-C coupling reactions catalyzed by palladium catalyst, it has been found the palladium nanoparticles are better stabilized in CN-IL compared to non-functionalized ionic liquids; thus enhanced catalytic activity and recyclability are realized.

Advantages of IL

Due to their non-volatility, effectively eliminating a major pathway for environmental release and contamination, ionic liquids have been considered as having a low impact on the environment and human health, and thus recognized as solvents for green chemistry. However, this is distinct from toxicity, and it remains to be seen how 'environmentally-friendly' ILs will be regarded once widely used by industry. Research into IL aquatic toxicity has shown them to be as toxic as or more so than many current solvents already in use. Available research also shows that mortality isn't necessarily the most important metric for measuring their impacts in aquatic environments, as sub-lethal concentrations have been shown to change organisms' life histories in meaningful ways. According to these researchers balancing between zero VOC emissions, and avoiding spills into waterways (via waste ponds/streams, etc.) should become a top priority. However, with the enormous diversity of substituents available to make useful ILs, it should be possible to design them with useful physical properties and less toxic chemical properties.

With regard to the safe disposal of ionic liquids it has been reported that the use of ultrasound to degrade solutions of imidazolium-based ionic liquids with hydrogen peroxide and acetic acid to relatively innocuous compounds is already practiced.
Despite their low vapor pressure many ionic liquids have also found to be combustible and therefore require careful handling. Brief exposure (5 to 7 seconds) to a flame torch will ignite these IL's and some of them are even completely consumed by combustion.
Ionic liquids are highly solvating, non-coordinating medium in which a variety of organic and inorganic solutes are able to dissolve. They are outstanding good solvents for a variety of compounds, and their lack of a measurable vapour pressure makes them a desirable substitute for VOCs. Ionic liquids are attractive solvents as they are relatively inexpensive to manufacture.

The key point about ionic liquids is that they are liquid salts, which means they consist of a salt that exists in the liquid phase and have to be manufactured, they are not simply salts dissolved in liquid. Usually one or both of the ions is particularly large in the case of ionic liquids. The low degree of symmetry of the cation will result in IL having a reduced lattice energy and hence with lower melting points. Special conditions are not usually required when carrying out reactions in neutral ionic liquids. For example, there is often no need to exclude water, or to carry out the reaction under an inert atmosphere. This, combined with the ability to design the ionic liquid to allow for easy separation of the product, makes reactions in ionic liquids extremely straightforward to carry out. Moreover, processes in ionic liquids do not require strictly anhydrous conditions or an inert atmosphere to carry out the reaction. This makes the whole reaction sequence easier, cheaper, and less time consuming to perform.

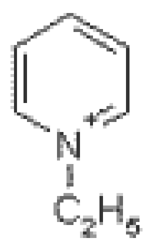
Disadvantages of IL

Extracting the chemical product from the ionic liquid in pure form can pose a problem. Water soluble compounds can easily be extracted with water and distillation can be used to separate compounds with high vapour pressure, however higher temperatures would be required to extract chemical products with low vapour pressures which will most likely result in the decomposition of the chemical product. Moisture sensitivity and the difficulty of separation of products containing heteroatoms are the difficulties encountered while using Ionic liquids.

Examples for typical IL cations

Cations such as substituted imidazoliums, substituted pyridiniums

Examples of an alkylpyridinium cation is shown below:



Examples of dialkylimidazolium cations are shown below:

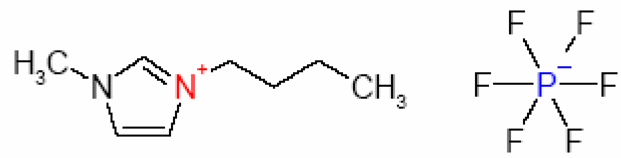
N-butyl pyridinium, 1-alkyl 3 –methylimidazolium cations

Examples for IL anions

Anions as borates, phosphates and halides and others Less common anions include: Triflate, Nonaflate, Bis trifylamide, Trifluoro acetate, Hepta fluoro butanoate etc.

Room Temperature Ionic Liquids

PF_6- for moisture stable water immiscible IL
BF_4- for moisture stable, but water miscible IL
Naming of IL can be done in the following way, including Cation Cation Anion Anion names in the respective order. For example, the following ionic liquid is named as 1-butyl-3-methylimidazolium hexafluorophosphate.



Chloroaluminate Ionic liquids

Acidic or basic IL can be obtained through varying the concentration of the following species

$Al_2Cl_7^- + Cl^- \rightarrow 2\ AlCl_4^-$

Acidic basic neutral

Large electrochemical windows are possible for both chloro and bromo ionic liquids. Basic haloaluminate in molten state preclude salvation and solvolysis of metal ion species. But they are moisture sensitive.

Applications:

Applications as solvents in

1. Catalysis
2. Synthesis
3. Electrochemistry
4. Separations

Recent activities in room temperature ionic liquids as solvents include:

Supercritical – CO_2 stripping after extraction, preparation of conducting RTIL, Ionic liquid polymer gel electrolytes, catalytic hydrogenation reactions, electrochemistry in RTIL, butene dimerisation, benzene polymerization, two phase separations, Friedel crafts regioselective alkylation and organometallic synthesis.

1. Catalysis

Reactant	Arene	Product	Yield (%)
Ferrocene	Benzene	$Fe(C_5H_5)(C_6H_6)$	53
Ferrocene	Toluene	$Fe(C_5H_5)(C_6H_5Me)$	64
Ferrocene	Naphthalene	$Fe(C_5H_5)(C_{10}H_8)$	53

IL can function both as catalyst and solvent. In a series of arene exchange reactions on ferrocene an acidic $[bmim]^+$ chloroaluminate IL was used where $[Al_2Cl_7]$- is the active Lewis acid. Lower yields observed for the solid arenes are eliminated in the case of RTIL.

2. Synthesis

Unique solvent effects may enhance the reaction rates in synthesis. Product selectivity can be enhanced by the nature of the anionic species.

Solvent	Conversion (%) Pent-1-ene	Yield (%)		TOF (mol/min)
		Pentane	Pent-2-ene	
Acetone	99	38	61	0.55
[bmim][SbF_6]	96	83	13	2.54
[bmim][PF_6]	97	56	41	1.72
[bmim][BF_4]	10	5	5	0.73

3. Electro Chemistry

Unique features of chloroaluminate ionic liquids include a large electrochemical window, although these anions are moisture sensitive. Possible applications include low cost and recyclable electrolytes for batteries, photochemical cells and electroplating. BF_4^- and PF_6^- ionic liquids have been developed as moisture stable electrolytes.

4. Separations

IL based method is a simple method for separations due to their water immiscibility. Ex: Pd (II) complexes in [bmim][BF_4] catalyze hydro dimerization of 1,3-butadiene. After the reaction, almost 97 % of the catalyst can be retained in the ionic liquid phase. RTIL is used as best alternatives to volatile organic solvents for liquid-liquid extractions. Benzene and derivatives partition to [bmim][Pf_6] from aqueous phase and may be selective. For example, *para* - hydroxyl benzoic acid and phthallic acid are soluble in [bmim] [BF_4] at a pH less than 2 where as aniline is soluble in the same IL at a pH greater than 10.

5. **Food science**

The application range of ionic liquid also extends to food science. For instance, [bmim]Cl (1-Butyl-3-methylimidazolium Chloride) is able to completely dissolve freeze dried banana pulp and the solution with an additional 15 % DMSO lends itself to Carbon-13 NMR analysis. In this way the entire banana compositional makeup of starch, sucrose, glucose, and fructose can be monitored as a function of banana ripening.

Future aspects of IL research:

As the green chemistry and IL originates at a single point, better utilizations for the social needs require a joint progress rather than their complimentary development. Insufficient knowledge in ionic liquids and the ignorance of its implications made this field empty without using its capabilities. Hence it is necessary to accumulate full information corresponding to IL for combinatorial development such as comprehensive tocxicity data, physical properties database, various existing chemistry, comparators for direct comparison of IL and other traditional solvents, industrial input into a research agenda, economic synthetic pathways and also a wider availability.

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