Accelerating Ionic Liquid Commercialization
Research Needs to Advance New Technology
June 2004
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Additional Information Available on the Vision2020 Web Site
(http://chemicalvision2020.org)


2. Ionic Liquids Reference List, Robin Rogers, University of Alabama

3. “Barriers to Ionic Liquid Commercialization” Workshop Presentations
   • Catalysis and Ionic Liquids, Jeff Miller, BP.
   • Overview: Technical Summaries on Ionic Liquids in Chemical Processing, David DePaoli, Oak Ridge National Laboratory.

4. “Barriers to Ionic Liquid Commercialization” Workshop Results, BCS, Incorporated
Executive Summary

Ionic liquids offer the potential for ground-breaking changes to synthesis routes and unit operations in the chemical industry. Essentially salts that are liquid at room temperature, their non-detectable vapor pressures and unique solvent properties provide the possibility for clean manufacturing.

There is rapidly growing worldwide scientific and commercial interest in ionic liquids, demonstrated by the accelerating number of ionic liquid publications and patents (Figure A). The prospects for ionic liquid use are vast. The literature and patents describe numerous applications such as catalysis with increased rates and yields, less complex and more energy-efficient separations, and solvents that may reduce environmental impacts for commercial processes (Exhibit A). The number of potential ionic liquids and liquid mixtures (estimated at $10^{18}$) gives research scientists a vast pool of candidates for synthesis. It should be possible to design an ionic liquid with specific properties to improve existing reaction and separation systems, or create entirely new routes and processes for chemical products. The substantial benefits described in the literature and patents should promote rapid ionic liquid technology adoption. Yet, despite their significant benefits and potential for numerous applications in the chemical industry, their development has remained mostly in the discovery stages of research. Industry has not been able to translate the benefits into viable industrial systems. Commercialization has been slow.

Seeking to investigate why ionic liquid commercialization has been slow, Chemical Industry Vision2020 Technology Partnership (Vision2020), an industry-led organization for accelerated innovation and technology development, formed a task force in December 2002 to identify potential industry-wide applications for ionic liquids and the key barriers to commercialization. Vision2020 recognized that an industry-wide effort to identify technical barriers and related research needs would quicken widespread commercialization of ionic liquids. The objective of the Vision2020 Ionic Liquid Task Force was to identify the key technical barriers that presently inhibit rapid and widespread commercialization of ionic liquids and develop recommendations to address these barriers. The approach was to gain a consensus of these technical challenges from industrial, academic, and government scientists active in ionic liquids research and related fields, and potential users of the technology. The goal was to develop specific research recommendations that would guide the allocation of resources towards collaborative industry-academic-government R&D programs designed to address these technical challenges.

Ionic Liquids

Ionic liquids are room temperature fluids composed entirely of ions, typically large organic cations and small inorganic anions. The thermodynamics and reaction kinetics of processes carried out in ionic liquids are different from those in conventional media. This creates new opportunities for catalytic reactions, separations, electrochemistry, and combined reaction/separation processes. Ionic liquids have no detectable vapor pressure and do not emit volatile organic compounds (VOCs), providing a basis for clean manufacturing – “green chemistry.”

Figure A: Worldwide Growth in Number of Ionic Liquid Publications and Patents

- Journals
- Patents

Year (*mid-2003)
The Vision2020 Ionic Liquid Task Force undertook a several-month effort that included a detailed literature and patent review (http://www.chemicalvision2020.org/), and a workshop, “Barriers to Ionic Liquid Commercialization,” that brought together a full range of chemical industry stakeholders.

The workshop was arranged in collaboration with the American Chemical Society (ACS) and followed a five-day Ionic Liquids: Progress and Prospects symposium (sponsored by Green Chemistry and Engineering and Separation Science and Technology Subdivisions) at the 226th ACS National Meeting (New York, Fall 2003). The “Barriers to Ionic Liquid Commercialization” workshop included thirty-six invited participants representing fifteen chemical companies, five universities, four non-governmental organizations, and three national laboratories. The facilitated workshop commentary is available at the Vision2020 Web site (http://www.chemicalvision2020.org/).

The Accelerating Ionic Liquid Commercialization report summarizes the task force’s efforts and defines specific R&D needs for ionic liquids. The commercialization barriers related to each application opportunity were similar, and are grouped into six categories: 1) process engineering, 2) environment, safety, and health, 3) economic benefit analyses, 4) fundamental understanding of compositional structure versus performance, 5) ionic liquid manufacturing, and 6) institutional issues. Multiple R&D efforts (Exhibit B) are recommended to surmount these barriers.

Targeted investments and a shared commitment among stakeholders are essential to attaining the ultimate goal of accelerated commercialization of innovative technology based on ionic liquids. To realize the commercialization potential of ionic liquids, U.S. stakeholders must invest in a new, solution-oriented approach to the development of ionic liquids and the chemical processes in which they could be used. This approach requires parallel efforts on (1) developing the fundamental understanding of ionic liquids so that they can be deliberately designed to meet industrial needs, and (2) applied research/development to prove that ionic liquids can be economically and safely manufactured and used in diverse chemical processes. This requires a robust understanding of the fundamental scientific principles involved in the synthesis of ionic liquids. Such an understanding will enable cost-effective design, synthesis, and scale-up of ionic liquid materials that deliver selected properties, allowing material producers to focus on the requirements for specific applications as the primary drivers of the design process. In addition, engineering-scale studies and pilot plant demonstrations are required to obtain the process engineering data needed to evaluate the technical and economic feasibility of industrial implementation of ionic liquid processes. These capabilities will accelerate ionic liquid development, moving the field from today’s discovery-based science to process development and application-based problem solving in the future. Once these capabilities become available, large numbers of diverse products could rapidly enter global markets to solve long-standing problems.
Recommendations:

- Perform engineering-scale studies to obtain the engineering data needed to support new efficient process designs that minimize the cost of utilizing ionic liquids and measure the technical performance and economic feasibility of industrial ionic liquid processes and new equipment designs.
- Obtain environment, safety, and health data on ionic liquids to access human health and environmental impact hazards, establish appropriate handling guidelines, and obtain regulatory acceptance.
- Perform research to obtain fundamental data, including physical properties relationships, to aid in rapid and efficient production of economical ionic liquids for use in industrial applications with extended lifetimes, high contamination tolerability, and low toxicity.
- Perform pilot plant demonstrations if economic benefit analyses warrant.

Exhibit B: Recommendations to Address Commercialization Barriers

**Process Engineering**
- Develop new efficient process designs that minimize the costs (volume) of ionic liquid systems.
- Perform process engineering studies on batch and continuous systems to determine ionic liquid lifetime performance, recovery, and reuse rates.
- Demonstrate ionic liquid performance with pilot-plant or semi-commercial scale projects.
- Determine impact of ionic liquid on end user product quality.

**Environment, Safety & Health**
- Determine impact on human health.
  - Perform early stage toxicology screening tests.
  - Establish transportation, handling and use guidelines.
- Assess ES&H impacts for ionic liquids and their breakdown products.
- Assess requirements (cost and time) and begin performing work required for TSCA (Toxic Substance Control Act) registration in United States and REACH (Registration, Evaluation and Authorisation of CHemicals) in European Union.

**Economic Benefit Analyses**
- Perform process economics studies for ionic liquid processes compared to traditional processes in use today.
- Perform economic benefit analyses for using ionic liquids in the chemical and allied industries.

**Fundamental Understanding of Compositional Structure versus Performance**
- Perform focused R&D to synthesize ionic liquids that meet important industrial parameters: increased lifetime, reduced costs, reduced toxicity, and increased contamination tolerability.
- Develop modeling and characterization tools to aid synthesis.
- Develop physical and chemical properties data (experimental measurement and prediction).

**Ionic Liquid Manufacturing**
- Develop robust and economic scale-up methods for industrial use of ionic liquids.
- Demonstrate reproducible production of high purity, high quality ionic liquids.

**Institutional Issues**
- Design and conduct workshops for industry that give a working knowledge of the chemistry, properties, and process design of ionic liquids.
- Develop strategic partnerships among industry stakeholders to accelerate commercialization through exchange of information and data on current and developing processes.
1. **Vision2020 Task Force**

*Chemical Industry Vision2020 Technology Partnership* (Vision2020) identified ionic liquids as an emerging technology that could significantly benefit the chemical industry by providing more efficient synthesis and processing systems, while at the same time lessening environmental impacts. Vision2020 believes that collaborative research efforts could accelerate implementation of this technology. In December 2002, Vision2020 organized a task force to address ionic liquid technology. The Vision2020 Ionic Liquids Task Force (*Appendix 1*) was assigned to identify key technical barriers to the commercialization of ionic liquids and develop specific recommendations for the research needed to address the barriers.

The Vision2020 Ionic Liquid Task Force recommended and Vision2020 authorized:

- A literature and patent review to focus on the application of ionic liquids to the chemical and allied industries (available at [www.chemicalvision2020.org](http://www.chemicalvision2020.org)) and,
- A workshop, “Barriers to Ionic Liquid Commercialization,” that would:
  1. Invite a range of chemical industry stakeholders in order to gain a broad consensus of the barriers to more rapid and widespread commercialization of ionic liquids,
  2. Identify the R&D needs with specific research recommendations to address these barriers, and
  3. Promote collaborative industry-academic-government R&D programs designed to address these technical barriers.

The literature and patent review was a state-of-the-art assessment of the technology completed by leading experts from universities and U.S. Department of Energy national laboratories (*Technical Summaries on Ionic Liquids in Chemical Processing*, available at [www.chemicalvision2020.org](http://www.chemicalvision2020.org)). This review confirmed the large number and rapid growth of published articles and patents (*Figure 1*) specifically addressing a broad range of catalysis and separation processes utilized in the chemical industry. Despite the reported attractive benefits of ionic liquids, development of industrial applications utilizing the unique properties of these fluids is limited and R&D efforts remain primarily associated with discovery-stage research. Industry does not yet view ionic liquids as a process alternative.

*Figure 1: Number of Ionic Liquid Catalysis and Separations Publications and Patents*
The Vision2020 Ionic Liquids Task Force, in order to gain a wide and reliable perspective on the barriers to ionic liquid commercialization, organized a workshop that brought together the key researchers, suppliers, and potential users. The workshop was planned in conjunction with the 226th American Chemical Society (ACS) National Meeting (New York, Fall 2003). This timing presented a unique opportunity to gather the fundamental researchers with applied production chemical engineers. The workshop followed a five-day Ionic Liquids: Progress and Prospects symposium (sponsored by Green Chemistry and Engineering and Separation Science and Technology Subdivisions). The symposium included ten technical sessions and more than eighty papers on ionic liquids. This symposium provided an extensive preview of the state-of-the-art in ionic liquids. The majority of papers focused on basic and exploratory ionic liquid research. However, one paper reported BASF AG’s successful use of an ionic liquid in a multi-ton batch separation process to produce a commercial product. BASF AG announced plans to convert to continuous operation and expansion to other processes (Exhibit 1.1). Other papers reported on ionic liquid processes that are emerging as potential commercial applications (Exhibit 1.2).

The Vision2020 Ionic Liquids Task Force workshop, “Barriers to Ionic Liquid Commercialization,” was held on September 11 and 12, 2003 (Appendix 2 - Agenda). Thirty-six invited participants (Appendix 3) from research organizations and industry met to identify barriers to the commercialization of ionic liquids. The participants represented fifteen chemical industry companies, five countries, five universities, four non-governmental organizations, and three U.S. Department of Energy national laboratories.

The workshop began with a presentation on the literature and patent review and with overviews from industry on the chemical process and product areas that may be impacted by ionic liquids (available at

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**Exhibit 1.1: Commercial Use of Ionic Liquids**

BASF is employing N-methylimidazolium chloride in the manufacture of alkoxyphenylphosphines – precursors for the synthesis of photoinitiators that are used in the manufacture of printing inks, as well as glass fiber and wood coatings.

Initial data indicates that the ionic liquid process produces a solvent-free product at a rate more than 100 times greater than the original process, with double the productivity.

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**Exhibit 1.2: Industrial Interest in Ionic Liquids is Rapidly Increasing**

- Development of Ionic Liquids Applications for ATOFINA Processes, P. Bonnet (ATOFINA).
- Deep Desulphurization of Fuels by Extraction with Ionic Liquids, A.Jess. (RWTH)
- Use of Ionic Liquids for Oil Shale Processing, M. Koel. (Tallinn Technical University)
- Novel Separation Processes Based on the Unique Solvation Properties of Ionic Liquids, S. Dai (ORNL), H. Luo, P. V. Bonnesen, A.C. Buchanan III.
The workshop focused on identifying commercialization barriers in two chemical process areas (catalyses and separations) and three broad chemical product areas (polymers, fuels, and bulk chemicals). The workshop was professionally facilitated to rapidly identify and prioritize the barriers to commercialization.

This report summarizes the work undertaken by the Vision2020 Ionic Liquids Task Force. It combines the background work and workshop results (available at www.chemicalvision2020.org) into Section 3, *R&D Needs to Address Ionic Liquid Commercialization Barriers*, and then suggests possible collaborative routes to overcome these barriers in Section 4, *The Path Forward*. 
2. Ionic Liquids Overview

Ionic liquids – salts having a melting point below 100°C – have recently attracted considerable worldwide attention as potential alternatives to conventional molecular organic solvents. They have application in a variety of catalysis, separations, and electrochemical processes. These solvents are composed entirely of ions, and strongly resemble ionic melts that may be produced by heating inorganic salts to high temperatures (800°C +). Many ionic liquids are highly polar and non-coordinating – ideal for catalytic reactions. Many are immiscible with water, saturated hydrocarbons, dialkyl ethers, and a number of common organic solvents – providing flexibility for reaction and separation schemes – and they are nonvolatile even at elevated temperatures. Since both the thermodynamics and kinetics of reactions carried out in ionic liquids are different from those in conventional media, they offer new and novel opportunities for catalytic reactions, separations, electrochemistry, and combined reaction/separation processes.

An ionic liquid generally consists of a large nitrogen-containing organic cation and a smaller inorganic anion. The asymmetry reduces the lattice energy of the crystalline structure and results in a low melting point salt. These simple liquid salts (single anion and cation) can be mixed with other salts (including inorganic salts) to form multi-component ionic liquids. There are estimated to be hundreds of thousands of simple ion combinations to make ionic liquids, and a near endless (10¹⁸) number of potential ionic liquid mixtures. This implies that it should be possible to design an ionic liquid with the desired properties to suit a particular application by selecting anions, cations, and mixture concentrations. Ionic liquids can be adjusted or tuned to provide a specific melting point, viscosity, density, hydrophobicity, miscibility, etc. for specific chemical systems.

The components of ionic liquids (ions) are constrained by high coulombic forces, and thus exert practically no vapor pressure above the liquid surface. Importantly, the near-zero vapor pressure (non-volatile) property of ionic liquids means they do not emit the potentially hazardous volatile organic compounds (VOC) associated with many industrial solvents during their transportation, handling, and use. (It should be noted, however, that the decomposition products of ionic liquids from excessive temperatures can have measurable vapor pressures.) In addition, they are non-explosive and non-oxidizing (nonflammable). These characterizations could contribute to the development of new reactions and processes that provide significant environmental, safety, and health benefits compared to existing chemical systems.
The scientific literature reports numerous chemical reactions in which ionic liquids are the media in which the reaction occurs. These include cracking, dissolution, hydrogenation, dimerization, isomerization, oligomerization, and other reactions. The ionic liquids used in a reaction or in catalytic systems are reported to show better activity, selectivity, and stability than traditional systems. They provide better yields, better and more controllable distribution of reaction products, and in some cases faster kinetics. Reactions in ionic liquids also occur at significantly lower temperatures and pressures than conventional reactions, resulting in lower energy costs and capital equipment costs. Ionic liquids can act as both catalyst and solvent. In many systems, the reaction products can be separated by simple liquid-liquid extraction, avoiding energy-intensive and costly distillation.
3. **R&D Needs to Address Ionic Liquid Commercialization Barriers**

Barriers to ionic liquid commercialization were identified through the task force and workshop efforts. They fall into six categories:

3.1 Process engineering,
3.2 Environment, safety, & health (ES&H),
3.3 Economic benefit analyses,
3.4 Fundamental understanding of compositional structure versus performance,
3.5 Ionic liquid manufacturing, and
3.6 Institutional issues.

The following sections describe these barriers, suggest ways to overcome them, and identify the research that would speed the widespread use of ionic liquids in the chemical industry.

### 3.1 Process Engineering

Chemical process engineering utilizes chemical property and thermodynamic data to design the process and build the equipment required to produce chemical products. Process engineering is both a science and an art. When, as in many cases, science does not give a complete answer, the process engineer must use experience and judgment to combine various sources of information into practical solutions to process design. Engineering-scale studies and pilot-plant demonstrations are the principal tools that provide the basis for experience and judgment decisions on the process design of new technologies. These studies and demonstrations, listed in Exhibit 3.1, are top research needs for the commercialization of ionic liquid systems. They will form the basis for more detailed and representative analyses of the economic, environmental, and other benefits attributed to ionic liquids in the published literature and patents (Section 3.3 Economic Benefit Analyses). These analyses will initially include many assumptions of system performance and operating costs. However, the studies and assumptions will lead to setting important performance and cost targets.

#### 3.1.1 Process Engineering Studies

Many of the ionic liquid studies to date have been performed at the laboratory scale under conditions that do not adequately represent operating conditions for full-scale industrial applications. Little information is publicly available on industrial processing equipment for reactors or separators incorporating ionic liquid processes. Therefore, one of the major obstacles that currently prevents widespread use of ionic liquids in the chemical industry is a lack of applied development studies to demonstrate that ionic liquids can be economically and safely used in diverse chemical processes.

A top priority research need is to perform engineering-scale studies to obtain performance data for side-by-side comparisons with traditional technologies and to provide valuable performance
data and scale-up parameters for fact-based evaluations of the technical and economic feasibility of industrial ionic liquid processes. The technical and economic feasibility studies will identify which ionic liquid applications potentially have commercial merit, and this information will provide direction to researchers working on synthesis and property characterization.

Solubility/equilibrium laws and entrainment phenomena can result in both loss of ionic liquids and contamination of ionic liquids during processing. Loss of ionic liquids to the aqueous phase has been noted during metal extraction in liquid-liquid systems. Dissolution of ionic liquids in aqueous or organic phases could present significant costs and waste-treatment challenges. New processes and equipment designs should be explored to reduce ionic liquid losses associated with solubility and entrainment phenomena.

Lifetime and recyclability data for ionic liquids is crucial to evaluating their viability in commercial applications. Ionic liquids may be sensitive to contaminants and may require frequent rejuvenation or replacement. The degree of sensitivity to impurities and the rate of degradation will have a large impact on ionic liquid functionality in industrial processes. Process engineering studies are required to obtain sufficient data on ionic liquid stability under long-term exposure to process conditions and exposure to air, moisture, heat, corrosion products, trace impurities (e.g., SO$_x$, NO$_x$, etc.) and other key industrial application components.

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### Exhibit 3.1: Research Requirements for Process Engineering

**Perform Process Engineering Studies**
- Demonstrate ionic liquid benefits by developing side-by-side comparisons with traditional chemical processes.
- Product selectivity, rate, and separation and other process performance capabilities.
- Determine useful lifetime of ionic liquids (life-cycle costs).
  - Determine impact of water content, sensitivity to contaminants, recycle, thermal stability, aging, ionic liquid losses, etc. over time.

**Develop Efficient Designs to Minimize the Costs of Processes Utilizing Ionic Liquids**
- Determine impact of properties, such as density, viscosity, solubilities, phase equilibria etc. on process design.
- Develop new reactor designs to maximize the benefits/performance of ionic liquids.
  - Develop new designs that focus on minimizing the volume of ionic liquid required.
- Develop, optimize, and demonstrate designs for ionic liquid processes under industrial conditions.
- Evaluate potential for retrofitting existing process equipment.
- Determine material-of-construction requirements.

**Perform Pilot-Plant and Large-Scale Demonstrations**
- Demonstrate ionic liquid benefits by developing side-by-side comparisons with traditional chemical processes.
- Validate smaller-scale technical and economic evaluation data.
- Obtain reliable scale-up data.

**Determine Impact of Ionic Liquid Processes on End-user Product Quality**
- Demonstrate that specifications for end products can be met (i.e., there are no unknown byproducts that could interfere with downstream customer applications).
Operational lifetimes have not been determined and these could impact the demand for and availability of ionic liquids. Ionic liquids that are too sensitive to contaminants or degrade under operating conditions may not be able to perform to the standards needed by industry. Demonstrated long-term stability and recyclability are vital for the economic viability of ionic liquids. Process engineering studies are also needed to obtain critical selectivity and rate data.

### 3.1.2 Equipment Design Parameters

Ionic liquids are a new process requiring new information to make the best practical designs for reaction or separation equipment. Designs for ionic liquid processes must be developed, optimized, and demonstrated under industrial conditions, taking into account unique ionic liquid properties. New process equipment should be designed to minimize the required volume of ionic liquid and reduce entrainment losses. Reduced inventory with efficient process design will lessen operating and capital costs and environmental, safety & health (ES&H) impacts associated with ionic liquid systems. The equipment in catalysis applications should be capable of removing desired reaction products from the ionic liquid without removing the ionic liquid itself. Non-traditional processing methods and equipment designs may yield more practical and economic systems to recover non-volatile solutes in ionic liquids, particularly salts.

When applied to production of existing chemicals, evaluations should be made to determine whether ionic liquid processes will require replacement of existing equipment or whether the equipment can be retrofitted to accommodate the new ionic liquid process. Engineering studies can determine if retrofitting existing plants and equipment can provide the process performance required or if new plants and equipment are needed to fully gain the benefits of ionic liquid technology. It is also necessary to determine materials-of-construction needs for ionic liquids. The need for new plants and equipment increases the expense and risk of using ionic liquid technology, especially when they displace existing (fully capitalized) plants and equipment. Many times, retrofits provide significant benefits at a reduced expenditure compared to new installations. This information will be required for the economic evaluations discussed in Section 3.3.

The equipment should be designed to minimize the required volume of ionic liquids through reduced inventory or efficient processing to reduce the cost and ES&H impacts associated with the process. The equipment should minimize the loss of the ionic liquids and be capable of removing desired reaction products from the ionic liquid without removing the ionic liquid in catalyst applications. For practical process development, non-traditional methods may be required to recover nonvolatile solutes in ionic liquids, particularly salts. Dissolution of ionic liquids in aqueous phase could also present significant cost and waste-treatment challenges. Loss of ionic liquids to the aqueous phase has been noted during metal extraction in liquid-liquid systems. New processes, such as supercritical phase splitting and water-structuring salts, may be required to reduce ionic liquid losses in aqueous streams.
3.1.3 Large-Scale Demonstration

A large-scale demonstration project would overcome one of the major barriers to the commercialization of ionic liquids – lack of performance data under industrial conditions. Well-documented and public demonstration(s) that can produce data on one or multiple commercial product streams under industrial operating conditions would be invaluable to promoting ionic liquid process. Pilot plant demonstrations are needed to:

- prove months-long continuous operation – including expected process upsets,
- determine the longevity of equipment in potentially harsh environments,
- verify compatibility of retrofitting existing equipment/facilities,
- obtain performance data for side-by-side comparisons with traditional technologies, and
- reduce the risk of using unproven technology.

With the information from various process engineering studies and demonstrations, the industry comfort level with ionic liquid technology will increase, and the longer-term benefits will become clear. Following the successful demonstration of scientific/physical capabilities, industry and researchers will be better able to creatively address cost issues and conduct cost-benefit analyses.

3.2 Environment, Safety & Health (ES&H)

Ionic liquids have no detectable vapor pressure and do not emit the volatile organic compounds (VOC) associated with many organic solvents (though the decomposition products from excessive temperatures can have measurable vapor pressures). Near-zero VOC emissions provide a basis for clean manufacturing – “green chemistry” – a highly desirable attribute for the chemical industry. However, each ionic liquid is likely to be classified as a “new chemical” and may require significant environment, safety & health (ES&H) studies prior to widespread use. Structural similarities between certain ionic liquids, herbicides and plant growth regulators have been noted. These similarities raise significant ES&H concerns and give ionic liquids a potentially large unknown risk factor. New health and safety concerns could also result from ionic liquid residuals in polymers, particularly those used for packaging food and personal care products.

Broad commercialization of ionic liquids will require a sound, science-based understanding of their environmental, safety, and health impacts. The development of exposure and handling guidelines for ionic liquid production, transportation, storage, use, and disposal are required. Generally accepted environmental, safety, and health protocols for ionic liquids will also have a significant impact in attracting employees to support accelerated scientific research, increasing manufacturer willingness to produce the materials, chemical manufacturer willingness to incorporate them in their production processes, and consumer willingness to buy products containing trace quantities of these materials.
Ionic liquid technology will benefit from addressing ES&H issues early along the commercialization pathway. While many ionic liquids may provide significant environmental benefits (reduced VOC), specific molecules, combinations, or classes of ionic liquids will need to be assessed for their toxicity, interaction/hazard reactivity data, stability data, and environmental migration information. Researchers and industry should work together to test, record, and evaluate these data. It may be possible to eliminate classes of ionic liquids that could not readily be used for ES&H reasons, and to focus research on the classes of ionic liquids that have acceptable risk. To determine the long-run ES&H benefits of ionic liquids, these studies should focus on comparison with the organic solvents that are in common use. Researchers, suppliers, and potential users of ionic liquids should work soon and closely with the appropriate regulatory agency to facilitate the registration process for those ionic liquids that are proven safe and effective (see Exhibit 3.2 for ES&H research requirements).

### 3.2.1 Toxicology, Environmental Impact, and Safety

While some environmental, safety, and health data can be applied broadly to classes of materials as an initial basis for internal handling and use protocols, it is often necessary to complete material specific studies before a chemical is regarded as “safe,” particularly when related to toxicity. The use of approaches similar to those currently employed by the chemical industry, and the use of existing knowledge and databases, is necessary to establish safety guidelines for ionic liquid research, production, and commercial application.

Today, knowledge is just emerging on the toxicity and environmental chemistry/transport of ionic liquids. Significant efforts are ongoing, both in obtaining toxicological data and in developing ionic liquids based on biomolecules (e.g., L-alanine ethyl ester hydrochloride) for reduced toxicity and increased biodegradability. Full toxicological data are available for one ionic liquid (PEG-5 cocomonium methosulfate), and others are being produced with low expected toxicity.

Researchers need to collect data on toxicity, interaction/hazard reactivity, stability, and environmental migration of ionic liquids and compare these data with traditional organic solvents. This work needs to begin as early as possible in the research phase in order to better target research efforts and reduce costs down the road. If the toxic, interaction/hazard reactivity, stability, and environmental migration properties of ionic liquids were better defined, it would

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**Exhibit 3.2: Research Requirements for Environment, Safety & Health Issues**

- **Assess human health and environmental impact hazards**
  - Study initial ionic liquid and potential breakdown products.
  - Determine toxicity and environmental impact.

- **Assess resources and time associated with the U.S. Toxic Substances Control Act (TSCA) and European Union REACH registration**
  - Work closely with regulatory agencies.

- **Determine exposure potentials for ionic liquids**
allow researchers to focus their development work on classes of ionic liquids that are acceptable, and eliminate classes that are viewed as high risk.

Extensive toxicity studies will need to be performed, especially when ionic liquids are to be used to remediate byproduct streams prior to disposal. Environmental safety is also an issue in certain chemical industry product lines, such as the polymers used in many food packaging and personal care products. These studies should include bioactivity, biodegradation, bioaccumulation, safety, health, interaction/hazard reactivity, stability, and environmental migration for both the initial ionic liquid and potential breakdown products.

3.2.2 Production Limits and Registration Costs

The United States and the European Union have regulatory limits on the production of new chemicals. Newly developed ionic liquids are likely to be classified as a “new chemical.” This may limit their availability. Developers, suppliers, and end users should work closely with regulatory agencies to ensure the timely production of ionic liquids for large-scale commercial use.

Production and use of ionic liquids in the United States is limited by the Toxic Substance Control Act (TSCA). TSCA section 5(h)(1) authorizes an exemption from Pre-Manufacturing Notice (PMN) requirements for new chemical substances manufactured for test marketing purposes, as long as this activity does not present an unreasonable risk to human health or the environment. The exemption would permit a company to assess the commercial viability of an ionic liquid and to receive customer feedback on product performance before proceeding with a PMN. A final revised rule in 1995 (USEPA 1995c) provided that new chemical substances may qualify for exemption from PMN if their annual production volume is less than ten metric tons. Manufacturers must submit exemption notices 30 days prior to commencement of manufacture. The ten metric ton limit may hinder early commercialization, as ionic liquid manufacturers go through the often lengthy and costly process of registering their product for higher production levels.

Under the new proposed EU regulatory framework REACH (Registration, Evaluation and Authorisation of CHemicals) chemical enterprises that manufacture or import more than one metric ton of a chemical substance per year would be required to register it in a central database. Registration would require describing the use and the intrinsic properties and hazards of each substance (such as physicochemical, toxicological and eco-toxicological properties). This proposed framework, like the TSCA could slow the manufacture of ionic liquids in the bulk quantities needed for large-scale industrial applications.

3.3 Economic Benefit Analyses

Ionic liquid applications that have broad chemical industry impact only become a reality when the economies of these applications are favorable and well understood. Detailed economic benefit analyses of ionic liquid processes are necessary and must be based on process
The costs of commercially using ionic liquids in industrial processes are unknown. Current published data do not allow for reliable extrapolation to broad industry application scale. The information and data developed from the research needs described in this report will begin to allow economic benefit analyses to be performed. Industrial process engineering groups need to perform cost-benefit analyses for industrial-scale ionic liquid processes: utilizing reliable capital costs, operating costs, and feedstock costs data. Side-by-side comprehensive cost-benefit analysis of direct and indirect advantages and risks of ionic liquid processes versus conventional technologies should be performed and published. Beyond a simple evaluation of the cost-benefit of ionic liquids in a specific process, these assessments should include estimates of long-term indirect benefits of ionic liquid use, such as water savings, energy savings, environmental benefits, the ability of an industry to be ahead of the market in terms of meeting or exceeding emissions standards, and other externalities that are not recognized when simply measuring the benefits of ionic liquids as a substitute for molecular solvents. This will provide a more comprehensive representation of how ionic liquids measure up to traditional organic solvent and catalytic systems.

Proper economic benefit analyses will help efficiently guide the direction of ionic liquid basic research (discovery and synthesis). They will also provide industry, government agencies, and other stakeholders with decision-making information. In addition, an early stage R&D screening process should be developed to guide future R&D efforts at improving return on investment and reducing the time to develop new ionic liquid processes.

### 3.4 Fundamental Understanding of Compositional Structure versus Performance

Basic and discovery research performed in academia or the national laboratories is often initiated by the investigator and based on a discovery approach. However, to successfully move basic and discovery research from a bench-top project to a commercial product, investments in research must focus on solving important industrial and/or societal problems (market pull vs. research push). Ionic liquid commercialization requires discovery researchers to not only develop fundamental understanding of ionic liquid synthesis and properties, but to impart these liquids with the chemical processing features needed for important industrial applications and markets.
Additionally, these newly developed ionic liquids must provide significant improvements over conventional technologies for them to be adopted by industry.

Developing an understanding of the reactions that form ionic liquids, ionic liquid chemical and physical properties, mechanisms/functions in catalysis and separation systems, and interactions with other materials (e.g., container vessels) is essential to their usefulness in industrial applications. Each ionic liquid that is developed has its own idiosyncrasies, each ion combination needs to be tested not only for its chemical and physical properties but for its reaction to impurities, toxicity, thermal stability, and its recyclability/long-term stability. Since the combinations of ions for potential ionic liquids are virtually endless, this is a monumental task.

It is estimated that there are hundreds of thousands of simple combinations of ions to make ionic liquids and a near endless ($10^{18}$) number of potential ionic liquid mixtures. This implies that it should be possible to design an ionic liquid for many, if not most, chemical systems. However, the search for synthesizing "the best" ionic liquids for given applications is a formidable challenge. Focused R&D will be required to accelerate commercialization of ionic liquids. Exhibit 3.4 lists the major research requirements for focused research in fundamental understanding of ionic liquids.

<table>
<thead>
<tr>
<th>Exhibit 3.4: Research Requirements for Fundamental Understanding of Structure versus Performance</th>
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<tbody>
<tr>
<td><strong>Predictive synthesis with an emphasis on practical industrial needs</strong></td>
</tr>
<tr>
<td>- Economic synthetic pathways</td>
</tr>
<tr>
<td>- Costs of raw materials and production of ionic liquid</td>
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<tr>
<td>- Lifetime of ionic liquid</td>
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<tr>
<td>- Toxicity of ionic liquid</td>
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<tr>
<td>- Contaminant tolerability</td>
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<tr>
<td>- Stability over a range of temperatures and water contents</td>
</tr>
<tr>
<td><strong>Physical and Chemical Properties: Measurement and Prediction</strong></td>
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<tr>
<td>- Physical properties</td>
</tr>
<tr>
<td>- Viscosity, density, vapor pressure, diffusion coefficients</td>
</tr>
<tr>
<td>- Thermodynamic, kinetic rates and chemical equilibrium properties</td>
</tr>
<tr>
<td>- Phase behavior: liquid-liquid-equilibria, liquid-gas-equilibria, partitioning coefficients</td>
</tr>
<tr>
<td>- Solubility parameters: miscibility, entrainment, effects of impurities</td>
</tr>
<tr>
<td><strong>Characterization Tools</strong></td>
</tr>
<tr>
<td>- Purity characterization methods</td>
</tr>
<tr>
<td>- High-throughput screening methods</td>
</tr>
<tr>
<td>- Combinatorial approaches to synthesis</td>
</tr>
<tr>
<td><strong>Modeling and Simulation to Aid in Synthesis</strong></td>
</tr>
<tr>
<td>- Properties prediction</td>
</tr>
<tr>
<td>- First-principles-based models for synthesis with desired chemical and physical properties</td>
</tr>
<tr>
<td>- Link between physical/chemical properties of ionic liquids or classes of ionic liquids and the performance in process systems</td>
</tr>
</tbody>
</table>
Toolkits based on fundamentals are needed for design and synthesis of ionic liquids with unique properties and to estimate the commercial merit of the ionic liquid in a target application. Laboratory-scale validation of performance must ensure that the ionic liquid will deliver the desired result when used in chemical processes to produce a variety of products. Therefore, developing links at the laboratory synthesis stage to processing engineering (Section 3.1), ES&H (Section 3.2), economic benefits analysis (Section 3.3), and ionic liquids manufacturing (Section 3.5) is extremely important. Research collaboration between the end user, the process engineers, materials manufacturer, the applications researchers, and the research chemists will be required to generate valid laboratory screening protocols.

3.4.1 First Principle Understanding of Ionic Liquid Synthesis Mechanisms

To accelerate ionic liquid commercialization, the investment in basic science must focus on developing predictive synthetic and property capabilities, solving important industrial and societal problems, and providing application-driven solutions not available with conventional technologies. Emphasis should be focused on developing ionic liquids with practical industrial needs in mind: economic synthetic pathways, minimizing costs of raw materials used to make ionic liquids, extended lifetime of the ionic liquid, minimum toxicity, and increased contaminant tolerability.

Production of ionic liquids in a controlled and predictable way for applications-driven research will require both a fundamental understanding of ionic liquid chemistry and new paradigms for synthesis. Fundamentals provide the rules of ionic liquid chemistry and physics that will enable synthesis of ionic liquids with predictable properties. Understanding the fundamental relationships between structure, properties, and reactivity will provide a foundation for significantly expanding ionic liquid development. Research of chemical groups or families of ionic liquids should be pursued. Development of fundamentals and methods of synthesis will require better physical and chemical properties data, characterization tools, and modeling breakthroughs as described below.

3.4.2 Chemical, Physical, and Thermodynamic Data

A fundamental understanding of the molecular level contributions to the unique properties of ionic liquids is required to allow “tunable” synthesis, to measure and to develop means to predict their physical and thermodynamic properties, and understand the reaction mechanisms involved when using ionic liquids as solvents and separating agents in chemical processes. Predicting properties is an exceedingly important capability in the synthesis of ionic liquids because compositions with lower functionality can be screened out before labor-intensive synthesis is attempted. Property measurement and prediction is essential both for guiding synthesis and for developing applications. A coupled experimental and theoretical approach should be undertaken.

Numerous physical and chemical property measurements are required for the synthesis, characterization and use of ionic liquids. These include: vapor-liquid equilibrium and liquid-liquid equilibrium in water and other solvents, conductivity, interfacial tension, thermal...
properties, diffusion coefficients, stability at elevated temperature and in multiphase environments, refractive index, density, viscosity, and others.

3.4.3 Characterization Tools

Ionic liquids cannot be analyzed directly by traditional gas chromatography (GC) or high-pressure liquid chromatography (HPLC). Development of rapid and efficient techniques for the analysis of ionic liquids is required to create ionic liquid property databases and quality control checks in industrial processes. Analysis of ionic liquids must be simple and reliable if ionic liquids are to be used as an alternative to conventional organic solvents.

Combinatorial chemistry methodology will be needed to conduct high-throughput synthesis and fast screening of ionic liquids. The data will be needed to determine the collective roles played by anions and cations for formation of room-temperature ionic liquids, to study what structural factors make such polar and charged molecules hydrophobic, and to explore stability, reactivity, and solvent properties. Investigation of these issues will lead to a better understanding of the ionic-liquid phenomenon, and ultimately to new classes of ionic liquids.

3.4.4 Modeling

Modeling and computational science could greatly aid in the prediction of properties and performance of ionic liquids. Synthesis of these materials based on the predictive design rules validates the understanding of fundamentals. Fundamental understanding of synthesis, mechanisms, and modeling are inextricably intertwined fields, and together they provide the foundation for ionic liquid manufacturing. Adopting this methodical, predictive approach based on fundamentals will accelerate development and applications. Predictive design is essential in order to address the increasing complexity of ionic liquid synthesis.

Modeling capabilities will provide greater flexibility for validating fundamentals based on experimentation. Ultimately, the capability to predict from first principles structure-property relationships will increase reliance on modeling and simulation, as required for cost-effective commercial production.

3.5 Ionic Liquid Manufacturing

Exhibit 3.5: Research Requirements for Ionic Liquid Manufacturing

Design and demonstration of ionic liquid manufacturing processes that provide:
- Robust and economic scale-up data for industrial volume cost projections
- Demonstrated reproducible production of consistent or high purity ionic liquids
Manufacturing of ionic liquids to date has primarily been done on a small scale. The ability to technically and economically scale up the manufacturing process needs to be demonstrated before ionic liquids will be used in industrial-scale volumes. Production of ionic liquids in a controlled, predictable, and consistent manner will require both a fundamental understanding of ionic liquid chemistry (Section 3.4) and possibly new paradigms for bulk synthesis. Ionic liquid manufacturing R&D needs are summarized in Exhibit 3.5.

### 3.5.1 Ionic Liquid Manufacturing Costs

Uncertainty of ionic liquid cost and availability for industrial chemical applications increases the risks associated with ionic liquid processes. Industry is unlikely to adopt this technology if the expenses of producing bulk ionic liquids remain at their current level (small laboratory quantities cost on the order of $1,000/kg). Even if the performance of ionic liquid processes is vastly superior, the costs associated with small losses of expensive ionic liquid inventory can quickly offset any processing benefit. The raw materials needed to produce many ionic liquids in quantities need for bulk chemical applications are not readily available and are reportedly expensive. No noteworthy published reports have been made that attempt to extrapolate the costs from small-scale research production to commercial-scale. There is a basic need for better understanding of ionic liquid synthesis, manufacturing processes and, very importantly, the economics associated with their manufacture. It is imperative that the research outlined in Sections 3.4.1, 3.1.2, and 3.1.1 are performed to synthesize less costly ionic liquids, develop new equipment designs to reduce the inventory of ionic liquids required in a process, and determine the practical ionic liquid lifetimes and potential loss rates. As these studies yield new and more reliable data to better measure the potential benefits of ionic liquids, economic benefit analyses outlined in Section 3.3 should be performed. These results should be used to guide further research to obtain economically viable ionic liquid processes.

### 3.5.2 Ionic Liquid Manufacturing Scale-up

Moving production from test tube to tank car quantities is never as simple as just a change of scale. Larger scale industrial manufacturing practices many times introduce new variables into the synthesis process and result in poorer quality, impure products. Ionic liquids researchers and process engineers need to demonstrate that ionic liquids can be scaled up from research to industrial quantities while maintaining their chemical and thermophysical properties and purity.

### 3.6 Institutional Issues

The path from discovery to commercial deployment of any new process or product is not smooth or straightforward, and many times is more successfully traveled when plotted backwards from commercial need to research concept (market pull vs. research push). Efficient information feedback loops along the path from discovery to commercialization are vital to overcoming and accelerating market adoption of any new process or product. Academic, government, and industrial collaborations, alliances, partnerships, and other joint ventures are known to
contribute to more efficient feedback loops and to accelerate the commercialization of new process and product technologies.

Lack of communication between industry and researchers limits the development rate of ionic liquids with potential commercial application. Industry has been slow to focus on the application of ionic liquids and slow to recognize their potential economic value. Ionic liquid researchers frequently lack insight into the specific details of industrial processes and applications. This fundamental disconnect between discovery researchers and industry is common to many new product and processes and contributes significantly to slow ionic liquid technology growth.

The question of where intellectual property rights reside is also a barrier to accelerating commercial use of ionic liquids. Each side of the equation, both developer and user, is understandably reluctant to work on a product without having ownership. Developers want to expand their market as rapidly as possible while users want to retain any competitive advantage they may have. Users also see an added risk in the vast number of potential ionic liquids. A user may have good intellectual property protection on one ionic liquid and/or process, but the vast number implies that there is likely to be more than one ionic liquid capable of providing a given performance.

Industry’s “business-as-usual” approach to building new or expanding processes entails using established solutions. Industry prefers to avoid the risks associated with new technologies, and frequently fails to recognize, understand, or investigate emerging technologies. Few industry researchers and engineering practitioners are involved in ionic liquids research, and technical knowledge is limited; the range of potential chemical industry applications has not been fully explored. This lack of basic process design studies and of demonstrated use prevents industry from even considering ionic liquids as potential substitutes for current processes. Even when informed of the theoretical benefits associated with ionic liquids, potential industry users remain reluctant to invest resources on processes that do not have an established track record.

Stakeholders should design and conduct workshops for the industry that give a working knowledge of the chemistry, properties and process design for ionic liquids. These workshops would broaden the knowledge and know how of potential ionic liquid users and the decision makers within the user organizations. These workshops may range from what is and is not known about ionic liquids and their application to forums that provide in-depth background data and information on a specific topic.

Strategic partnerships among a subset of industry stakeholders can also accelerate the commercialization of ionic liquids. Partnerships can be developed under non-disclosure agreements (NDAs) to address intellectual property concerns and discuss opportunities, capabilities, and define the roles for each participant. Partnerships between researchers and specific industry sectors needing replacement of current solvents or technologies will allow for an exchange of information and data on the current processes and the eventual development of new processes.
4. The Path Forward

This report provides the reader with a realization and measure of the R&D work that remains to be accomplished before ionic liquids are considered a viable alternative to conventional catalytic and separation technologies for producing moderate and large volume products. Despite the attractive promise of new efficient and “green” processes based on ionic liquids, development of industrial processes utilizing the unique properties of these fluids has been hampered by the barriers described earlier. A major objective of Vision2020 Task Force initiative is to promote collaborative industry-academic-government R&D programs to address technical barriers. Strategies and funding approaches for high priority R&D are given in Exhibit 4.1.

Chemical industry stakeholders should begin work as early as possible in areas appropriate for collaborative research. These areas include:

1. **Process Engineering User Facilities**: Stakeholders should evaluate the merit of establishing a facility or facilities at a national laboratory or university that would, for a fee, be open to all for use in performing process engineering and equipment design studies needed to support new efficient process designs that minimize the cost of utilizing ionic liquids and measure technical performance and economic feasibility of industrial ionic liquid processes and new equipment design. The facilities would allow interested parties to develop the process engineering data required to move forward with
commercialization without having to invest the entire capital required for demonstration. The facility staff would provide broad expertise for the more rapid development of industrial projects using ionic liquids.

2. **Environmental, Safety and Health (ES&H):** All aspects of ES&H (toxicology, bioactivity, bioaccumulation, ecological impacts, environmental impacts, storage, handling, etc.) need to be addressed for ionic liquid use. The very limited data and information available to date are not adequate for ionic liquids to move beyond the research stage. This is important work both from a commercial and societal aspect. This work would greatly benefit from collaborative efforts and the early involvement of regulatory agencies. An early determination should be made on the practicality and regulatory acceptance of focusing ES&H studies on families or specific categories of ionic liquids.

3. **Focused Fundamental Research to Increase Industrial Focus and Obtain Chemical, Physical, and Thermodynamic Properties Data:** Industry-guided research in fundamental understanding of ionic liquids should focus on industrial application-based problem solving aimed at production of low-cost ionic liquids with extended lifetimes, high contamination tolerability, and low toxicity for use in industrial applications. Universal access to the chemical, physical and thermodynamic properties of ionic liquids is needed to accelerate development and use of ionic liquids. Collaboratively funded research rapidly distributes results to the broad ionic liquid community. Existing mechanisms to distribute properties data include The International Union of Pure and Applied Chemistry (project 2003-020-2-100) ionic liquids database and the American Institute of Chemical Engineers’ Design Institute for Physical Properties (DIPPR).

4. **Economic Benefit Analyses:** Economic benefit analyses should be performed to set performance targets for future research and to quantify the benefits of ionic liquids compared to current technology. These analyses are a major driver in the commercialization process. They need to be integrated with fundamental research, process engineering, and ionic liquid manufacturing studies.

5. **Large-Scale Demonstrations:** If economic benefit analyses warrant, demonstrate ionic liquids at one or more commercial sites with industrial users willing to share performance data and design information. Large-scale or semi-commercial-scale demonstrations not only provide valuable engineering data but are an important mechanism for lowering the perceived risks of new technology. Results of government-funded demonstrations should be made publicly available, but intellectual property rights/concerns may limit participation by some potential industrial users.

Vision2020 will distribute this report among its members and provide it to chemical industry stakeholders. Its goal is that this report acts as a lens for members and stakeholders to better focus R&D resources to ionic liquid commercialization. It is important to recognize that the
information, know how, needs, and resources for moving from research concept to a commercial use seldom reside in one organization. The R&D barriers identified can be eased or overcome more rapidly when researchers, suppliers, users, and other stakeholders join in collaborative efforts. The institutional barriers can be eased with information exchanges and workshops that allow stakeholders to share their knowledge and experience. Vision2020 will define this report a “success” if it encourages and hastens the collaborations, alliances, partnerships, workshops, and other joint ventures needed to accelerate research aiding the widespread commercialization of ionic liquids.
# Appendix 1: Vision2020 Task Force Members

<table>
<thead>
<tr>
<th>Team Member</th>
<th>E-mail</th>
<th>Phone</th>
<th>Organization</th>
</tr>
</thead>
<tbody>
<tr>
<td>Francis Via</td>
<td><a href="mailto:Thevias@oco.net">Thevias@oco.net</a></td>
<td>914-962-5583</td>
<td>Vision 2020, Fairfield Resources</td>
</tr>
<tr>
<td>Emory Ford</td>
<td><a href="mailto:eaford@comcast.net">eaford@comcast.net</a></td>
<td>413-584-0512</td>
<td>Vision 2020, Materials Technology Institute</td>
</tr>
<tr>
<td>Sharon Robinson</td>
<td><a href="mailto:Robinsonsm@ornl.gov">Robinsonsm@ornl.gov</a></td>
<td>865-574-6779</td>
<td>Vision 2020, Oak Ridge National Laboratory</td>
</tr>
<tr>
<td>Bill Choate</td>
<td><a href="mailto:bchoate@wcs-hq.com">bchoate@wcs-hq.com</a></td>
<td>410-997-7778</td>
<td>BCS, Incorporated</td>
</tr>
<tr>
<td>Marc Villegas</td>
<td><a href="mailto:marc.villegas@mba.wfu.edu">marc.villegas@mba.wfu.edu</a></td>
<td>336-782-0032</td>
<td>BCS, Incorporated</td>
</tr>
<tr>
<td>Neil Stephenson</td>
<td><a href="mailto:neil_stephenson@praxair.com">neil_stephenson@praxair.com</a></td>
<td></td>
<td>Praxair</td>
</tr>
<tr>
<td>Keith Hutcheson</td>
<td><a href="mailto:Keith.w.hutcheson@usa.dupont.com">Keith.w.hutcheson@usa.dupont.com</a></td>
<td>302-695-1389</td>
<td>Dupont</td>
</tr>
<tr>
<td>Jeff Miller</td>
<td><a href="mailto:Millejt1@bp.com">Millejt1@bp.com</a></td>
<td>630-420-5818</td>
<td>bp</td>
</tr>
<tr>
<td>Mike Ford</td>
<td><a href="mailto:fordme@apci.com">fordme@apci.com</a></td>
<td>610-481-4284</td>
<td>Air Products</td>
</tr>
<tr>
<td>Roger Moulton</td>
<td><a href="mailto:Rmoulton@sacheminc.com">Rmoulton@sacheminc.com</a></td>
<td>512-912-4408</td>
<td>Sachem</td>
</tr>
<tr>
<td>Conrad Zhang</td>
<td><a href="mailto:Zongchao.zhang@akzo-nobel.com">Zongchao.zhang@akzo-nobel.com</a></td>
<td>914-679-5304</td>
<td>Akzo Nobel</td>
</tr>
<tr>
<td>Prof. Joan Brennecke</td>
<td><a href="mailto:jfb@darwin.helios.nd.edu">jfb@darwin.helios.nd.edu</a></td>
<td>574-631-5847</td>
<td>University of Notre Dame</td>
</tr>
<tr>
<td>Prof. Robin Rogers</td>
<td><a href="mailto:rdrogers@bama.ua.edu">rdrogers@bama.ua.edu</a></td>
<td>205-348-4323</td>
<td>University of Alabama</td>
</tr>
<tr>
<td>Dr. David DePaoli</td>
<td><a href="mailto:depaolidw@ornl.gov">depaolidw@ornl.gov</a></td>
<td>865-574-6817</td>
<td>Oak Ridge National Laboratory</td>
</tr>
<tr>
<td>Dennis Dees</td>
<td><a href="mailto:Dees@cmt.anl.gov">Dees@cmt.anl.gov</a></td>
<td>610-252-7349</td>
<td>Argonne National Laboratory</td>
</tr>
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</table>
Appendix 2: Barriers to Ionic Liquid Commercialization Workshop Agenda

September 11, 2003

Riverside Ballroom
5:00 - 6:00 PM Reception & Refreshments
6:00 - 6:10 PM Welcoming Remarks and Introductions
   Emory Ford
   Materials Technology Institute
6:10 - 6:30 PM Overview of Technology Summaries &
   Literature
   David DePaoli, Ph.D.
   Oak Ridge National Lab
6:30 - 6:50 PM Overview Presentation – Catalysis
   Jeff Miller, Ph.D.
   BP Chemical
6:50 - 7:10 PM Overview Presentation – Separations
   Jeff Kanel
   J.S. Kanel & Associates, LLC
7:10 - 7:30 PM Path Forward
   Roy Tiley
   BCS, Incorporated

September 12, 2003

Riverside Ballroom
7:00 - 7:45 AM Continental Breakfast
7:45 - 8:00 AM Introduce Facilitators and Instructions
8:00 - 10:20 AM Breakout Sessions: Chemical Processes:
   Catalysis
   Separations
   • What are the chemical process barriers to commercial use of Ionic
     Liquids?
   • What are the key chemical process barriers to commercialize Ionic
     Liquids?
   • What are the strategies to overcome these Barriers?
   • What order must these strategies occur to successfully overcome the
     barriers?
   • Who are the R&D players/supporters in chemical processes?
10:20 - 10:40 AM Break
10:40 - 12:15 PM Breakout Session: Product Applications:
   Polymers
   Fuel Production
   Bulk Chemicals
   • What are the product application barriers to commercialized use of Ionic
     Liquids?
   • What are the key product application barriers to commercialize Ionic
     Liquids?
   • What are the strategies to overcome these Barriers?
12:15 - 1:15 AM  Lunch
1:15 – 2:10 PM  Breakout Session Continued: **Product Applications: (Polymers, Fuel Production, and Bulk Chemicals)**
  - What order must these strategies occur to successfully overcome the barriers?
  - Who are the R&D players/supporters in product applications?
2:10 – 2:20  Break
2:20 - 3:00 PM  Summary and Wrap-up
3:00 PM  Adjourn
Appendix 3: List of Workshop Participants

Martin Atkins  
BP Chemicals  
atkinsmp@bp.com

Philip Alexander Barrett  
Praxair Inc.  
philip_barrett@praxair.com

Joan Brennecke  
University of Notre Dame  
jfb@nd.edu

Suk-Ku Chang  
C-TRI  
csk9018@chol.com

Bill Choate  
BCS, Incorporated  
bchoate@bcs-hq.com

Sheng Dai  
Oak Ridge National Laboratory  
dais@ornl.gov

Liese Dallbauman  
Gas Technology Institute  
liese.dallbauman@gastechnology.org

James Davis  
University of South Alabama  
jdavis@jaguar1.usouthal.edu

David DePaoli  
Oak Ridge National Laboratory  
depaolidw@ornl.gov

Mark Dietz  
Argonne National Laboratory  
mdietz@anl.gov

Michael Driver  
ChevronTexaco Corporation  
mdriver@chevronexaco.com

Emory Ford  
Vision2020, Materials Technology Institute  
eaford@comcast.net

Joe Gardner  
National Starch and Chemical  
joseph.b.gardner@nstarch.com

Winfried Geissler  
Merck KgaA, Germany  
winfried.geissler@merck.de

Martin Grendze  
Reilly Industries, Inc.  
mgrendze@reillyind.com

Mark Harmer  
DuPont  
Mark.A.Harmer@usa.dupont.com

Robert T. Hembre  
Eastman Chemical Company  
rhembre@eastman.com

Nikolai Ignatiev  
Merck KgaA, Germany  
nikolai.ignatiev@merck.de

Carsten Jost  
Degussa AG  
carsten.jost@degussa.com

Jeffrey Kanel  
J. S. Kanel & Ass., LLC  
jskanel@charter.net

Joe Kocal  
UOP LLC  
joseph.kocal@uop.com

Edward Maginn  
University of Notre Dame  
ed@nd.edu
Chris Marshall  
Argonne National Laboratory  
marshall@cmt.anl.gov

Jeff Miller  
BP Chemicals  
millejt1@bp.com

Phillip Rakita  
Armour Associates, Ltd.  
perakita@aol.com

Sharon Robinson  
Vision 2020, Oak Ridge National Laboratory  
robinsonsm@ornl.gov

Robin Rogers  
The University of Alabama  
RDRogers@UA.EDU

Martin Schiller  
DuPont  
martin.schiller@usa.dupont.com

Jan Seetz  
Akzo Nobel Chemicals  
jan.seetz@akzonobel.com

Michael Stoll  
Los Alamos National Laboratory  
mstoll@lanl.gov

Francis Via  
Vision2020, Fairfield Resources  
via@frlicense.com

Peter Wasserscheid  
Solvent Innovations  
The Aachen University of Technology  
wasserscheid@itmc.rwth-aachen.de

Masayoshi Watanabe  
Yokohama National University  
mwatanab@ynu.ac.jp

Urs Welz-Biermann  
Merck KgaA, Germany  
urs.welz-biermann@merck.de

Conrad Zhang  
Akzo Nobel Chemicals  
zongchao.zhang@akzonobel-chemicals.com

Peter Wasserscheid  
Solvent Innovations  
The Aachen University of Technology  
wasserscheid@itmc.rwth-aachen.de

Masayoshi Watanabe  
Yokohama National University  
mwatanab@ynu.ac.jp

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