230th American Chemical Society Meeting & Exposition
August 28 – September 1, 2005 Washington, DC

IUPAC Ionic Liquids Database - ILThermo

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Outline

- Background Information
- ILThermo Database Organization
- Ionic Liquids Specification
- Web Presentation

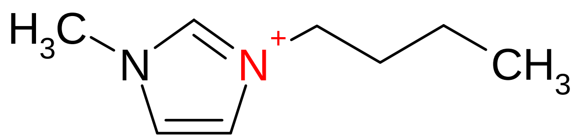
What are Ionic Liquids (ILs) ?

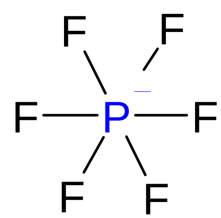
- ILs are salts that melt below 100^{o}C, composed wholly of ions.
  - CATIONS such as substituted imidazoliums, substituted pyridiniums or others
  - ANIONS such as borates, phosphates and halides and others

- Naming examples and structures

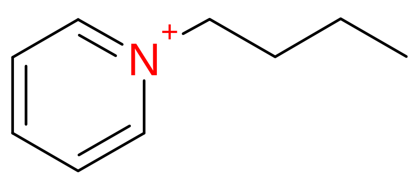
CATION **ANION**

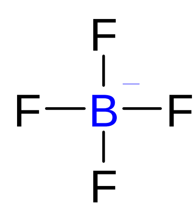
(1) 1-butyl-3-methylimidazolium hexafluorophosphate





(2) N-butylpyridinium tetrafluoroborate





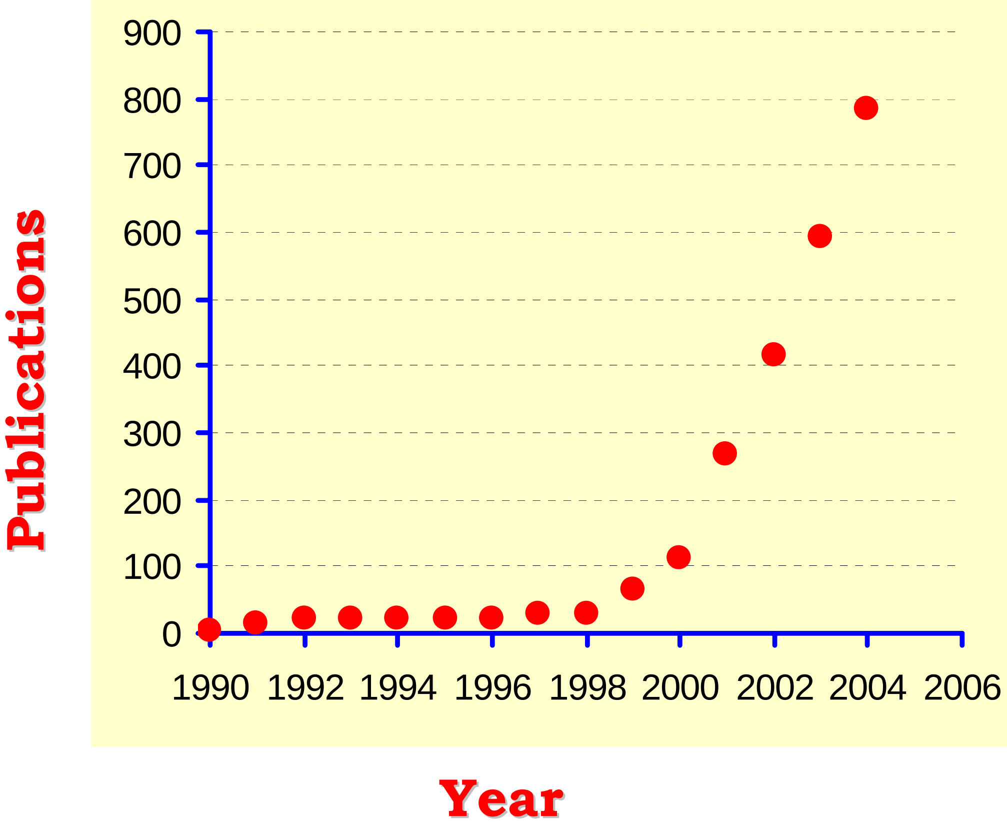
Why are ILs a Hot Topic ?

- ***The materials are unique (properties and variety)***
  - *Tunability*
  - *Negligible vapor pressure*
  - *Good thermal stability*
  - *Wide liquid range*
  - *Electrolytic conductivity*

- ***The prospects for ILs applications are vast***
  - ***Possibility to establish environmentally benign chemical processing***
    - *20 million ton VOCs discharged into atmosphere per year*
    - *2/3 of all industrial emission and 1/3 of VOCs emission nationwide from traditional solvents*
    - *Global climate change, poor urban air quality, and human illness*
  - ***Potential to revolutionize the way how solvents are utilized***
    - *New extraction, catalysis, separations , and polymer processes*
    - *New chemical synthesis*
    - *Enhancement of existing processes*
  - ***Opportunities to develop task-target performance chemicals***
    - *Engineering fluids for machinery and equipment*
    - *New materials in the automotive, textile, construction, oil and gas, and energy industries*

Dramatic Increase in Research on Ionic Liquids

Worldwide Escalation in Number of Ionic Liquids Publications (Web of Science)



Year	Publications
1990	3
1991	15
1992	21
1993	22
1994	20
1995	23
1996	21
1997	29
1998	30
1999	64
2000	112
2001	266
2002	417
2003	592
2004	786
Total	**2421**

Workshops and Conferences

2000

NATO Advanced Research Workshop – "Green Industrial Applications of Ionic Liquids" in Heraklion, Crete, Greece with 41 participants

2001 – 2003

Trilogy of American Chemical Society (ACS) National Meeting Ionic Liquid Symposia in San Diego, 2001, Boston, 2002, and New York, 2003

2002

Workshop on Ionic Liquids: Properties of Ionic Liquids and their Application in Chemical Engineering. IACT/IUPAC International Conference on Chemical Thermodynamics, Rostock, Germany

2003

Ionic Liquids Symposium, in Melbourne, Australia

2004

Ionic Liquids Workshop of Background, State-of-the-Art, and Academic/Industrial Applications in The University of Alabama, Tuscaloosa, AL

2005

1st International Congress on Ionic Liquids in Salzburg, Austria. More than 400 participants from 33 countries and six continents

1st International Congress on Ionic Liquids

Overall:

279 presentations

Main Topics:

- *New ionic liquids – synthesis of ionic liquids*
- *Characterization and thermodynamic properties and modeling*
- *Toxicology, persistence and sustainability*
- *Interesting new applications in synthesis, catalysis, biocatalysis, separation, electrochemistry and analytics*

Thermodynamic Property Data:

- *72 presentations*
- *26% of total presentations*

Message from the Salzburg Congress

Opportunities

- *Storage and delivery of hazardous gases like phosphine or BF_3*
- *Detect ethanol by using ILs as solvents for advanced NMR-techniques*
- *ILs based electrolytes for dye-sensitized solar-cells and for the deposition of metals*
- *Suitable solvents for the dimerization of olefins*

Challenges

- *Cost of ILs and ILs technology*
- *Complexity of coordination, speciation, and extraction in chemical processes when utilizing ILs*
- *Limited information and data on structural variations, chemical and physical properties, corrosion and toxicity.*

Urgent Call for Data

"A public, free, independently verified, web-based database of physical, thermodynamic, and related data is urgently needed. There is also an immediate need for toxicity, biodegradation, bioaccumulation, and other safety, health, and environmental impact data. New analytical tools are also required for assessing the purity of ionic liquids. In addition, applications-oriented research on ionic liquids should include cost-benefit, economic, and life-cycle analyses."

Professor Robin D. Rogers
Center for Green Manufacturing
The University of Alabama
"Green Industrial Applications of Ionic Liquids"
NATO Advanced Research Workshop, April, 2000

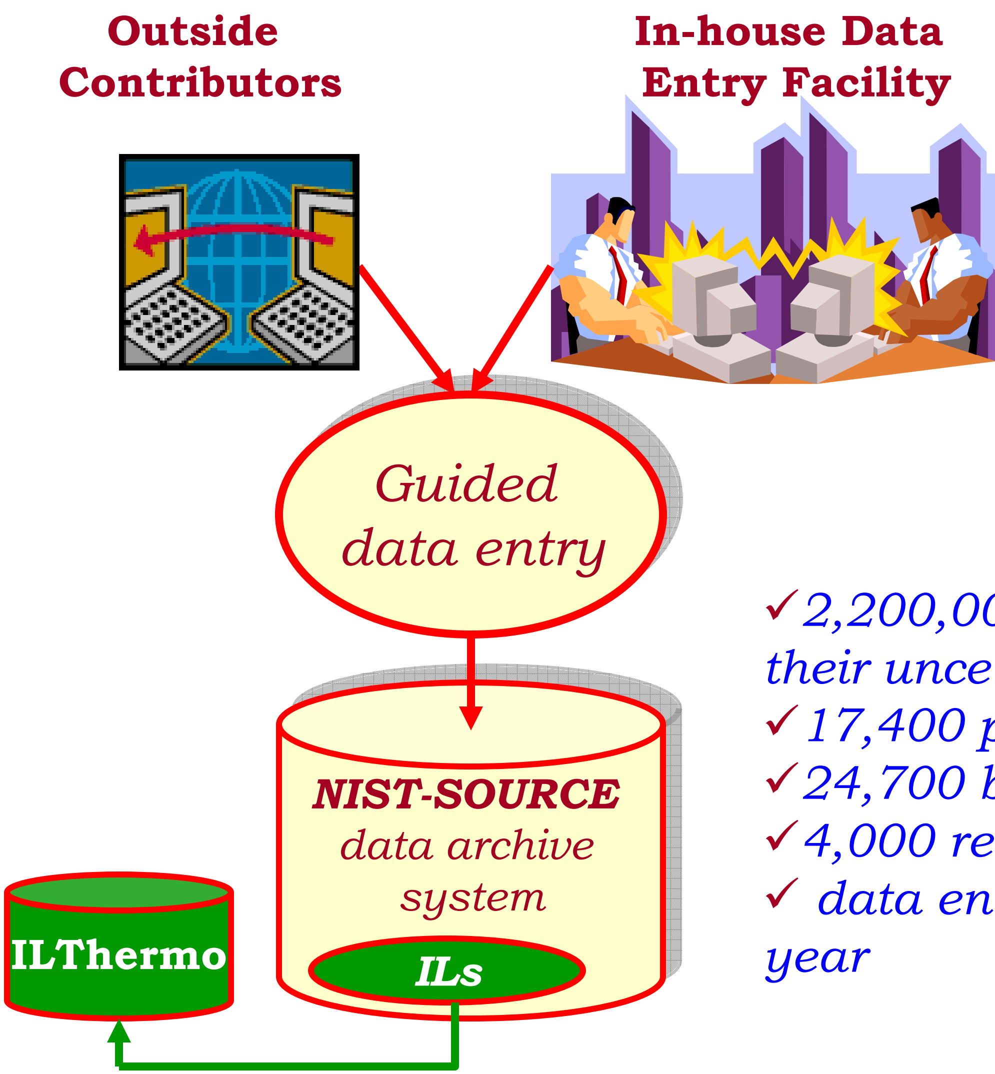
Two IUPAC Task Groups on Ionic Liquids Data

- *Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems at http://www.iupac.org/projects/2002/2002-005-1-100.html, formed in 2002.*
  - *Encourage systematic studies of thermodynamic and thermophysical properties*
  - *Recommend a reference ionic liquid and make reference quality measurements*
- *Ionic liquids database at http://www.iupac.org/projects/2003/2003-020-2-100.html, formed in 2003*
  - *Create a new database of experimental thermodynamic properties for ionic liquids*
  - *Provide a web-based comprehensive data retrieval system with free public access*

IUPAC Ionic Liquids Database - ILThermo

- ***Aim***
  - *Provide users worldwide with an up-to-date collection of experimental investigations on ILs*
- ***Subject Coverage:***
  - *Chemical identification of ions and ILs*
  - *Chemical systems of pure ILs, binary and ternary mixture systems containing ILs*
  - *Thermodynamic, thermochemical and transport properties*
  - *Phase behavior and solvent properties*
  - *Sample purity*
  - *Metadata (state variables, phases, system constraints, and measurement technology…)*
  - *Reviews and bibliography*
- ***Developments and Plans***
  - *Develop and maintain at NIST as an ongoing commitment*
  - *Provide FREE public access*
  - *Anticipated public release for December of 2005*

NIST-SOURCE for ILs Depository and Data Entry



NIST-SOURCE

Depository of all experimental thermophysical and thermochemical properties reported in the world's scientific literature

Include

✓2,200,000 numerical property values and their uncertainties

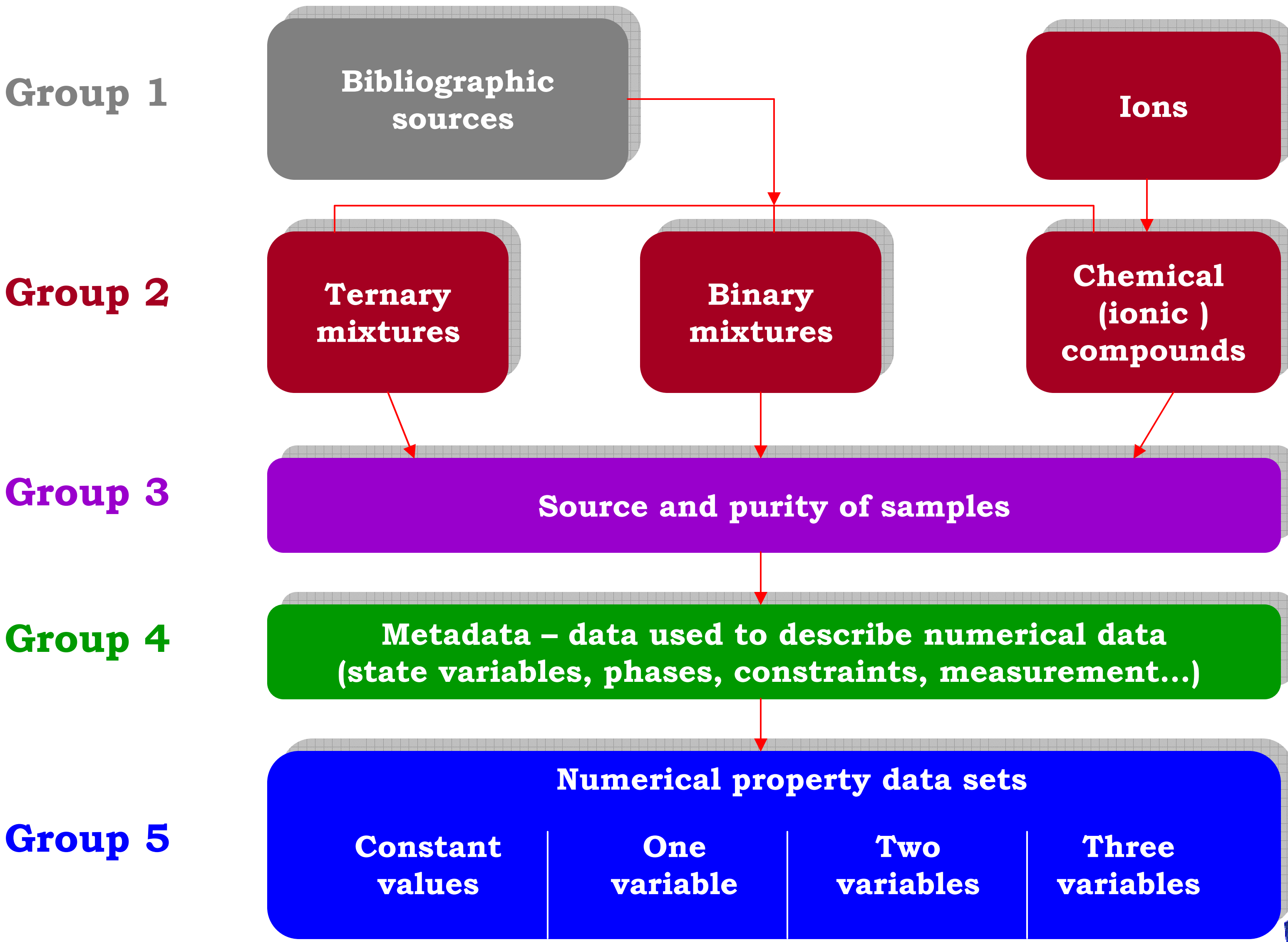
✓17,400 pure compounds

✓24,700 binary and ternary mixture systems

✓4,000 reaction systems

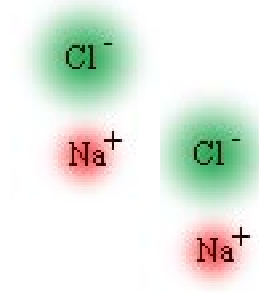
✓ data entry rate is near 300,000 values per year

ILThermo Database Organization



Specifications for ILThermo Database

- *Ions*
- *Ionic liquids*
- *Relation of ions and ionic liquids*
- *Pure ionic compounds*
- *Binary mixtures containing ionic liquids*
- *Ternary mixtures containing ionic liquids*
- *Measurement technology*
- *Sample purity*
- *Physiochemical property data*
- *Uncertainty*



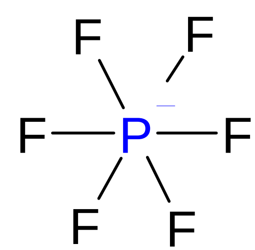
Identification of Ions

Each cation or anion is identified by:

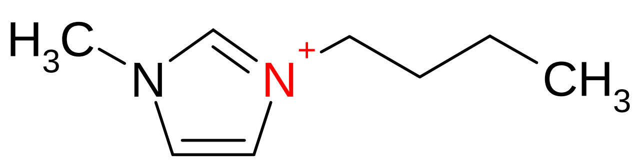
- *Chemical Abstract Registry number*
- *Ionic formula*
  - *the simplest ratio of cation and anion; not discrete entities*
- *Ionic charge*
  - *positive charge for cation and negative charge for anion*
- *Name*
- *Structure*

Examples

ANION – ***CASRN:*** *16919-18-9* ***Formula:*** PF_6 ***Charge:*** *-1*
Name: *Hexafluorophosphate*



CATION – ***CASRN:*** *80432-08-2* ***Formula:*** $C_8H_{15}N_2$ ***Charge:*** *1*
Name: *1-Butyl-3-methylimidazolium*



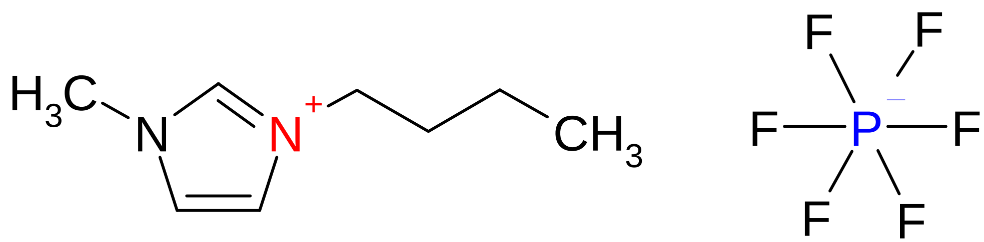
Identification of Ionic Liquid

AN IONIC COMPOUND *is represented in the same way as other chemical substances.*

- *Chemical Abstract Registry number*
- *Molecular formula*
- *Molecular weight*
- *Name*
- *Molecular structure*

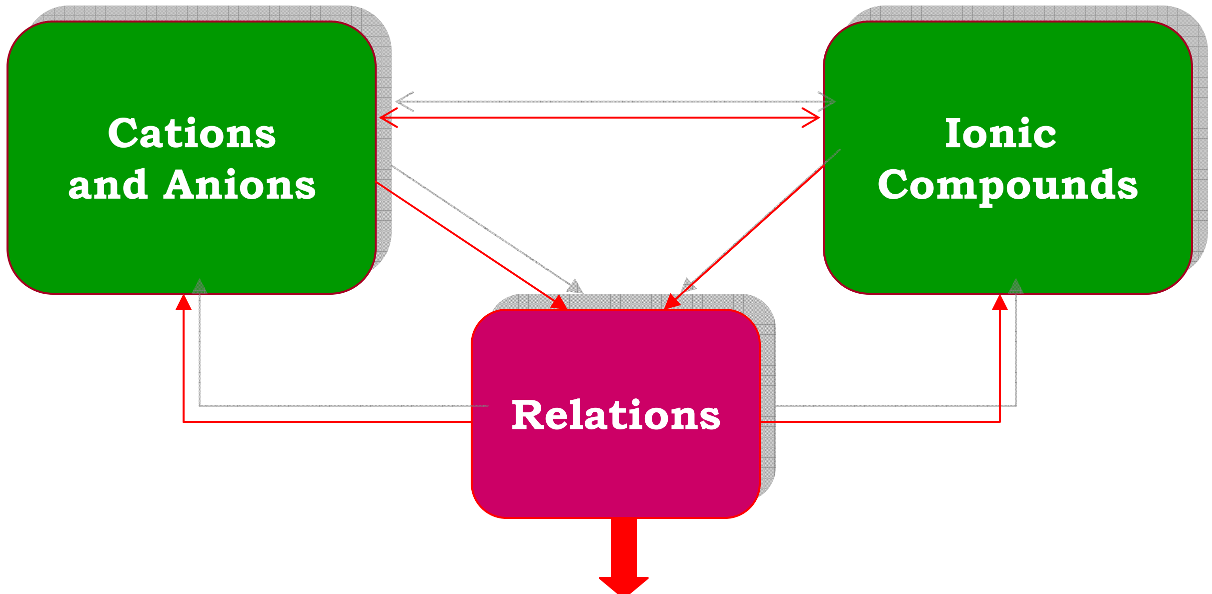
Example

IONIC LIQUID – ***CASRN:*** *174501-64-5* ***Formula:*** $C_8H_{15}F_6N_2P$
Molecular weight: *284.18*
Name: *1-butyl-3-methylimidazolium hexafluorophosphate*



CATION *– 80432-08-2, C8H15N2, 1-butyl-3-methylimidazolium*
ANION *– 16919-18-9, PF6 , Hexafluorophosphate*

Relation of Ions and Ionic Compounds



- *For any selected cation or anion, there are links to all ionic compounds containing this ion*
- *For any selected ionic compound, there are links to all ions constituting this ionic liquid*

Chemical Systems of Ionic Liquids

❖ ***Pure ionic compounds***

Cation + anion

❖ ***Binary mixtures containing ionic liquids***

Ionic liquid + molecular compound

Molecular compounds: (a) water; (b) alcohols; (c) aliphatic alkanes; (d) cyclohydrocarbons; (e) aromatic hydrocarbons; (f) chloroalkanes; and (g) CO_2 and other gases

Examples:

- *Solubility of oxygen and carbon dioxide in 1-butyl-3-methyl imidazolium tetrafluoroborate*
- *Apparent molar volume and isentropic compressibility of ionic liquid 1-butyl-3-methylimidazolium bromide in water, methanol, and ethanol*

❖ ***Ternary mixtures containing ionic liquids***

Examples:

- *Conductivities and viscosities of the ionic liquid [bmim][PF_6] + water + ethanol and [bmim][PF_6] + water + acetone*
- *Ionic liquids/water distribution ratios of some polycyclic aromatic hydrocarbons*

Sample Purity

1) **Original Source of the Sample**
   Standard reference sample; Commercial source; Synthesized by author; Isolated from a natural product; not stated

2) **Initial Purity of sample**
   Reported at a percentage of mole percent or mass percent; water and halid impurity identified

3) **Method of purification**
   21 common methods identified such as adsorption of impurities, crystallization, a chemical reagent, fractional distillation …

4) **Final purity of sample**

5) **Method of Purity Analysis**
   13 methods identified such as chemical analysis, density, differential scanning calorimeter, mass spectrometry, NMR …

Physicochemical Property Data

- ***Data Type***

  Strict application of the Gibbs Phase Rule (GPR) forms the basis for organizing numerical data in the database. The number of independent variables, called degree of freedom of the system given by GPR, is a fundamental criteria used to classify all types of physicochemical properties as:
  - *Constants (critical temperature and pressure)*
  - *with one state variable (heat capacity – Temperature T)*
  - *with two state variables (solubility – T, Composition X)*
  - *with three state variables (viscosity – T, X and Pressure P)*

- ***Data Set***

  Each data set / data point in the database consists of two parts:
  - *metadata (identification of chemical components, phases, units, constraints, chemical composition, state variables, measurement purpose and method …)*
  - *numerical data (values of state variables, property, and the estimated uncertainty)*

Data Uncertainty (1)

***J. Chem. Eng. Data* 2005, 50, 546-550**
Uncertainty Reporting for Experimental Thermodynamic Properties
Qian Dong, Robert D. Chirico, Xinjian Yan, and Michael Frenkel

"Estimates of uncertainty are the measure of data quality for all experimentally determined quantities and form the basis for the understanding, evaluation, and application of all scientific data.

…

Although few scientists would disagree that the reporting of reliable uncertainty information is important, it is broadly recognized that the nature and extent of that reporting in the literature is highly variable".

Data Uncertainty (2)

1. Source and purity of sample
2. Measurement technique limits
3. Calibration of instruments
4. Care used to perform the measurement
5. Completeness and adequacy of description of procedure
6. Agreement among duplicate measurements, or between measurements on standard samples and other accepted values
7. Special effect such as contamination or decomposition of sample
8. Estimates of uncertainty, precision, or reproducibility given by the investigator
9. Experience and credibility of the investigator

Web Presentation of Physicochemical Property Data for Ionic Liquids

ILThermo Database Main Menu

http://132.163.193.215:8989/ILNov27_1-ViewController-context-root/intronew.uix

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IUPAC Ionic Liquids Database is an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structures, properties, and uses.

Property Data for Ionic Liquids

Ions | Ionic Liquids | Property | Literature

Property Data for Binary Mixtures Containing Ionic Liquids

Ions | Ionic Liquids | Property | Literature

Property Data for Ternary Mixtures Containing Ionic Liquids

Ions | Ionic Liquids | Property | Literature

Search Ions or Ionic Liquids

Ions | Ionic Liquids

About Search Methods

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NIST

Search Criteria

Ions
- CASRN
- Formula
- Charge
- Names

Ionic Liquids
- CASRN
- Formula
- Molecular weight
- Names

Property
- Category
- Description

Bibliography
- Author's name
- Journal title
- Article title
- Year of publication

To be added
- Measurement method
- Sample purity
- Other statistics

How to Search A Piece of Data by Ions ?

Reference:

Title: Thermochemistry of ionic liquid heat-transfer fluids

*Authors: M. E. **Van Valkenburg**, R. L. Vaughn, M. Williams and J. S. Wilkes*

Source: Thermochim. Acta 425 (2005) 181-188

Ionic liquid studied:

Name: 1-ethyl-3-methylimidazolium tetrafluoroborate

CASRN: 143314-16-3

Formula: $C_6H_{11}BF_4N_2$

Measurements of :

- ***Heat capacity at constant pressure***
- *Specific density*
- *Triple point temperature*
- *Thermal conductivity*
- *Viscosity*
- *Normal melting temperature*
- *Enthalpy of Transition*

Total 16 property data sets

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Thermochimica Acta 425 (2005) 181–188

thermochimica acta

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Thermochemistry of ionic liquid heat-transfer fluids☆

Michael E. Van Valkenburg, Robert L. Vaughn, Margaret Williams, John S. Wilkes*

Department of Chemistry, 2355 Fairchild Drive, Suite 2N225, US Air Force Academy, CO 80840-6230, USA

Received 4 June 2004; received in revised form 1 September 2004; accepted 6 September 2004
Available online 15 December 2004

Abstract

Large-scale solar energy collectors intended for electric power generation require a heat-transfer fluid with a set of properties not fully met by currently available commercial materials. Ionic liquids have thermophysical and chemical properties that may be suitable for heat transfer and short heat term storage in power plants using parabolic trough solar collectors. Ionic liquids are salts that are liquid at or near room temperature. Thermal properties important for heat transfer applications are melting point, boiling point, liquidus range, heat capacity, heat of fusion, vapor pressure, and thermal conductivity. Other properties needed to evaluate the usefulness of ionic liquids are density, viscosity and chemical compatibility with certain metals. Three ionic liquids were chosen for study based on their range of solvent properties. The solvent properties correlate with solubility of water in the ionic liquids. The thermal and chemical properties listed above were measured or compiled from the literature. Contamination of the ionic liquids by impurities such as water, halides, and metal ions often affect physical properties. The ionic liquids were analyzed for those impurities, and the impact of the contamination was evaluated by standard addition. The conclusion

http://132.163.193.215:8989/ILNov27_1-ViewController-context-root/intronew.uix

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Property Data for Binary Mixtures Containing Ionic Liquids

Ions | Ionic Liquids | Property | Literature

Property Data for Ternary Mixtures Containing Ionic Liquids

Ions | Ionic Liquids | Property | Literature

Search Ions or Ionic Liquids

Ions | Ionic Liquids

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Privacy Statement

http://132.163.193.205:8989/ILThermoJuly28-ViewController-context-root/pureions.uix.do

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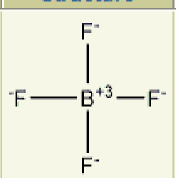
By ions | By Compounds | By Property | By literature

Search property data by Ions

To browse ions, select entries in the following tables OR start new search with search criteria [Search]

Available Cations or Anions:

Select	CASRN	Formula	Ionic Charge	Ionic Names
(•)	14874705	BF4	-1	Borate(1-), tetrafluoro- ; Fluoroborate; Tetrafluoroborate; Tetrafluoroborate (BF41-); Tetrafluoroborate anion; Tetrafluoroborate(1-);
○	24959679	Br	-1	Bromide ; Bromide (Br-); Bromide anion; Bromide ion; Bromide ion (Br1-); Bromide ion(1-); Bromide(1-); Bromine ion; Bromine ion(1-); Bromine(1-); Bromine, ion (Br1-); Hydrobromic acid, ion(1-);
○	98837980	C2F6NO4S2	-1	Bis(perfluoromethylsulfonyl)imide; Bis(trifluoromethylsulfuryl)imide; Methanesulfonamide, 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-, ion(1-) ;
○	37181398	CF3O3S	-1	Methanesulfonic acid, trifluoro-, ion(1-) ; Triflate; Triflate anion; Triflate ion ((CF3SO3)-); Trifluoromethanesulfonate; Trifluoromethanesulfonate ion; Trifluoromethanesulfonate(1-); Trifluoromethanesulfonic acid ion(1-); Trifluoromethylsulfonate;
○	16887006	Cl	-1	chloride ion;
○	16919189	F6P	-1	Hexafluorophosphate; Hexafluorophosphate ion; Hexafluorophosphate(1-); Hexafluorophosphate(1-) ion; Phosphate(1-), hexafluoro- ;
○	85100829	C10H19N2	1	1-Hexyl-3-methylimidazolium; 3-Hexyl-1-methylimidazolium; 1H-Imidazolium, 1-hexyl-3-methyl- ;
○	178631033	C12H23N2	1	1H-Imidazolium, 1-methyl-3-octyl- ;
○	45428103	C16H31N2	1	1H-Imidazolium, 1-dodecyl-3-methyl-;
○	45470324	C5H9N2	1	1,3-Dimethylimidazolium; 1H-Imidazolium, 1,3-dimethyl- ;
○	65039034	C6H11N2	1	1-Ethyl-3-methylimidazolium; 1-Methyl-3-ethylimidazolium; 1H-Imidazolium, 1-ethyl-3-methyl- ; 3-Ethyl-1-methylimidazolium;
○	131097159	C7H13N2	1	1,2-Dimethyl-3-ethylimidazolium; 1-Ethyl-2,3-dimethylimidazolium; 1H-Imidazolium, 1-ethyl-2,3-dimethyl- ;
○	80432082	C8H15N2	1	1-Butyl-3-methylimidazolium; 1H-Imidazolium, 1-butyl-3-methyl- ;
○	157310708	C8H15N2	1	1,2-Dimethyl-3-propylimidazolium; 1H-Imidazolium, 1,2-dimethyl-3-propyl- ;
○	45806959	C9H14N	1	1-Butylpyridinium; Pyridinium, 1-butyl-;
○	108203890	C9H17N2	1	1-Butyl-2,3-dimethylimidazolium; 1H-Imidazolium, 1-butyl-2,3-dimethyl- ; 3-Butyl-1,2-dimethylimidazolium;

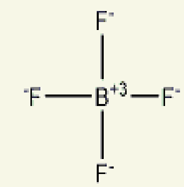
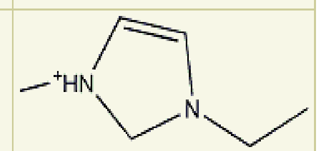
CASRN	Structure
14874705	

http://132.163.193.205:8989/ILThermoJuly28-ViewController-context-root/pureions.uix.do

Ionic liquid(s) Containing the Ion - 14874705

Select	CASRN	Chemical Formula	Molec.Weight	Ionic Liquid Name
(•)	143314163	C6H11BF4N2	197.97	1-ethyl-3-methylimidazolium tetrafluoroborate; 1H-imidazolium, 1-ethyl-3-methyl-, tetrafluoroborate(1-) ; [EMIM][BF4];
( )	174501656	C8H15BF4N2	226.03	1-butyl-3-methylimidazolium tetrafluoroborate; 1H-imidazolium, 1-butyl-3-methyl-, tetrafluoroborate(1-) ; [BMIM][BF4];
( )	203389280	C9H14BF4N	223.02	N-butylpyridinium tetrafluoroborate; pyridinium, 1-butyl-, tetrafluoroborate(1-) ;
( )	244193508	C10H19BF4N2	254.08	1-hexyl-3-methylimidazolium tetrafluoroborate;
( )	244193520	C12H23BF4N2	282.13	1-methyl-3-octylimidazolium tetrafluoroborate; 1-octyl-3-methylimidazolium tetrafluoroborate;

Ions constituting the ionic liquid - 143314163

CASRN	Formula	Ionic Charge	Ionic Name	Structure
14874705	BF4	-1	Borate(1-), tetrafluoro- ; Fluoroborate; Tetrafluoroborate; Tetrafluoroborate (BF41-); Tetrafluoroborate anion; Tetrafluoroborate(1-);	
65039034	C6H11N2	1	1-Ethyl-3-methylimidazolium; 1-Methyl-3-ethylimidazolium; 1H-Imidazolium, 1-ethyl-3-methyl- ; 3-Ethyl-1-methylimidazolium;	

Available Properties for the Ionic Liquids - 143314163

Select	Property Category	Description	References	Data Points
(•)	Heat Capacity	Heat capacity at constant pressure, J/(K.mol)	1	14
( )	Phase Change Enthalpy	Enthalpy of transition or fusion, kJ/mol	1	1
( )	Thermal Properties	Thermal conductivity, W/(m.K)	1	10
( )	Transport Properties	Viscosity, Pa.s	2	8
( )	Temperature	Normal freezing point, K	1	1
( )	Volumetric Properties	Specific density, kg/m**3	2	8

Data Summary

Property: Heat capacity at constant pressure, J/(K.mol)
Compound: Name - 1-ethyl-3-methylimidazolium tetrafluoroborate; 1H-imidazolium, 1-ethyl-3-methyl-, tetrafluoroborate(1-) ; [EMIM][BF4];
CASRN - 143314163 Formula - C6H11BF4N2
Total References: 1
Total Data Points: 14

References and Data Sets

Select	Year Pub.	Authors	Data Set	Data Type	Variable1	Variable2	Phase1	Phase2	Phase3
⦿	2005	Van Valkenburg, M. E.; Vaughn, R. L.; Williams, M.; Wilkes, J. S.	1	One Variable	Temperature, K		Liquid		

Purity and Measurement

Source: Synthesized by the author
Initial Purity: Not stated
Purification: Not stated
Final Purity: 99 mol %, .065water mass %.113 halide impurity mass %
Purity Analysis: Spectroscopy, kf Acid-base titration

Measurement Purpose: Direct observation
Measurement Method: Small sample (50 mg) DSC

Selected Data Set (Property/Uncertainty - Heat capacity at constant pressure, J/(K.mol))

Year Pub.	Data Set	Temperature, K	Property Value	Uncertainty
2005	1	273.1	244.492	4.949
2005	1	283.1	247.462	4.949
2005	1	293.1	250.036	4.949
2005	1	303.1	252.213	4.949
2005	1	313.1	253.995	5.147
2005	1	323.1	255.579	5.147
2005	1	333.1	256.767	5.147
2005	1	343.1	257.558	5.147
2005	1	353.1	258.152	5.147
2005	1	363.1	258.152	5.147
2005	1	373.1	257.954	5.147
2005	1	383.1	257.361	5.147
2005	1	393.1	256.569	5.147
2005	1	403.1	255.183	5.147

Selected Reference

Year Pub.	Authors	Source
2005	Van Valkenburg, M. E.; Vaughn, R. L.; Williams, M.; Wilkes, J. S.	Thermochim. Acta 425 , 181-188

Title: Thermochemistry of ionic liquid heat-transfer fluids

Keywords: Ionic liquid; Heat capacity; Heat transfer; Thermal conductivity; Thermal stability

Abstract: Large-scale solar energy collectors intended for electric power generation require a heat-transfer fluid with a set of properties not fully met by currently available commercial materials. Ionic liquids have thermophysical and chemical properties that may be suitable for heat transfer and short heat term storage in power plants using parabolic trough solar collectors. Ionic liquids are salts that are liquid at or near room temperature. Thermal properties important for heat transfer applications are melting point, boiling point, liquidus range, heat capacity, heat of fusion, vapor pressure, and thermal conductivity. Other properties needed to evaluate the usefulness of ionic liquids are density, viscosity and chemical compatibility with certain metals. Three ionic liquids were chosen for study based on their range of solvent properties. The solvent properties correlate with solubility of water in the ionic liquids. The thermal and chemical properties listed above were measured or compiled from the literature. Contamination of the ionic liquids by impurities such as water, halides, and metal ions often affect physical properties. The ionic liquids were analyzed for those impurities, and the impact of the contamination was evaluated by standard addition. The conclusion is that the ionic liquids have some very favorable thermal properties compared to targets established by the Department of Energy for solar collector applications.

Anticipated Functionality from ILThermo

- ***Provide users worldwide with free internet access to literature information on experimental investigations on ionic liquids***

- ***Assist researchers in their literature search, data evaluation, systematic studies on the direction of future investigations***

- ***Allow chemical engineers access to complete and up-to-date physicochemical property data of ionic liquids***