Reviews

ILThermo: A Free-Access Web Database for Thermodynamic Properties of Ionic Liquids†

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The development, scope, and functionality of the Web-based ionic liquids database, ILThermo, are described. The database is available free to the public and aims to provide users worldwide with up to date information from publications of experimental thermophysical properties for ionic liquids, including numerical property values, measurement methods, sample purities, purification methods, and uncertainties. The database can be searched in terms of the ions constituting the ionic liquids, the ionic liquids themselves, and their properties and through literature citation information

Introduction

In 2003, the IUPAC (International Union of Pure and Applied Chemistry) Project *Ionic Liquids Database* (Task Group Chairman, Kenneth R. Seddon; Project 2003-020-2-100)[1] was initiated with the objective: "Create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses; lack of this information is impeding progress in a burgeoning field of significant current interest." This article describes the principal product of this project, the NIST ILThermo Database[2] for thermophysical properties of ionic liquids, as well as their binary and ternary mixtures with other compounds.

The dramatic increase in published research on ionic liquids over the last 5 years is shown in Figure 1, where values for the figure were compiled with a search for the term "ionic liquid" in titles, keywords, and abstracts using the Web of Science from 1990 through 2006. The search yielded 4800 articles, nearly a third of which were published in 2006. The special characteristics that have made ionic liquids attractive to the scientific and engineering communities, particularly their possible use as solvents to replace volatile organics, are well-known.[3]

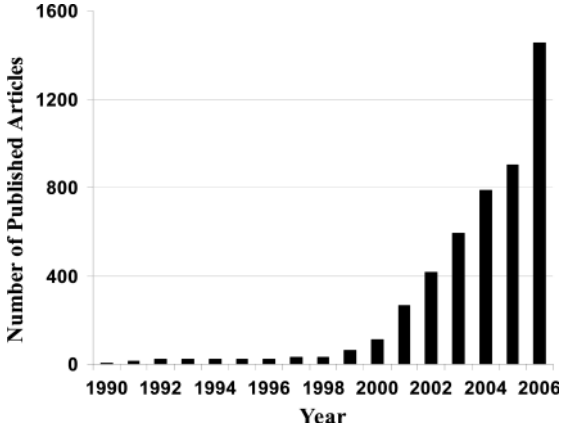

Figure 1. Number of journal articles related to ionic liquids published yearly.

In addition to the general interest in ionic liquids, the database was established to bring together essentially all of the experimental data for these materials to allow a comprehensive critical evaluation of the properties. Through trial and error, researchers have learned that some properties of ionic liquids are very sensitive to trace amounts of water and other impurities. Consequently, full sample descriptions are an important component of the database design. Indeed, recognition of this problem led to establishment in 2002 of the IUPAC project *Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems* (Task Group Chairman, Kenneth N. Marsh; Project 2002-005-1-100).[4]

A key goal of the *Ionic Liquids Database* project was to create a living database, continuously updated with the experimental thermodynamic properties of ionic liquids from the worldwide scientific literature. In addition to structured data compilation and presentation, an initial critical evaluation for each value

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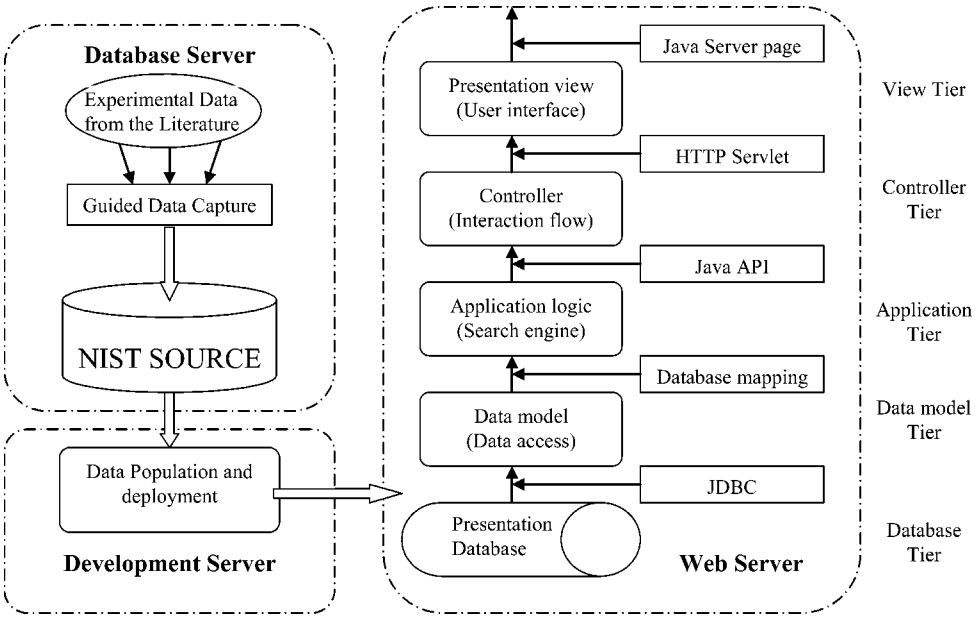


Figure 2. Overview of ILThermo major development and deployment components.

was to be included. In order to make this goal a reality in a timely manner, the task group members decided to create a new ionic liquids database, entitled ILThermo, utilizing the existing data framework, the NIST TRC SOURCE Data Archival System (SOURCE).[5] SOURCE is an extensive repository system of experimental thermophysical and thermochemical property data for pure components, binary and ternary mixtures, and chemical reactions extracted from the scientific literature and currently contains nearly 3 million data points on over 18 000 pure substances, 25 000 binary mixtures, 5000 ternary mixtures, and 4000 chemical reactions. SOURCE is utilized to support the production of evaluated and selected data in both print and electronic formats required for a variety of technical applications at NIST.

Overview of the ILThermo Web-Based Application

The ILThermo database system was developed, and is deployed and maintained, through the three major servers shown in Figure 2. These are (1) an ORACLE transactional database server for in-house data collection from the literature with NIST Guided Data Capture software,[6] data storage, and data evaluation; (2) a DELL workstation as a development server for transforming the subset of SOURCE used to create ILThermo; and (3) a public Web server to provide worldwide access to ILThermo.

In the database server section, data collection and storage have been accomplished by extending SOURCE to accommodate ionic liquids and their component ions. Extensions were also made to include specific purity descriptors, such as halide and water content, in addition to overall compound purity. Comprehensive extraction and storage in SOURCE of the world's thermodynamic data is an active long-term project at NIST. With SOURCE at the core of data collection and management for ILThermo, a stable and living data compilation for the scientific community is assured. In this development model, ILThermo, a presentation-oriented database, is designed, created, and automatically populated to meet the requirements of physicochemical data search tasks for ionic liquids. An N-Tier architectural design has been implemented that contains five major tiers: (1) presentation database, (2) data model, (3) application logic, (4) controller, and (5) view, as shown at the right side of Figure 2.

The main features of the ILThermo Web-based application are summarized here. Detailed lists of the thermophysical properties presently included in the scope of ILThermo are listed in Table 1 for pure ionic liquids, binary mixtures, and ternary mixtures. General property groups are listed in column 1, while specific properties are listed in column 2. Property groups are used to make location of a specific property easier for the user. In general terms, ILThermo provides:

- A primary archive of experimentally measured thermophysical property data values for ionic liquids from the published literature
- Rigorously defined numerical values with full and clear specification of all variables, constraints, phases, and properties
- Detailed metadata for key elements in the experimental investigations, such as sample purities, purification methods, and property measurement methods
- Uncertainty for each measured property value as estimated by the database producers
- Up to date information on ionic liquids publications from major scientific journals
- Comprehensive Web-based data presentation through a series of Master/Detail data views

In addition to being a historical record, envisioned usages of the database include service as a resource for experimental investigators, as a source of original data for evaluators and compilers, and as a convenience for all users of property data, including process engineers and academics.

The server architecture used to deploy the N-Tier database viewing system is centered on a RedHat Linux ES 4 two-node cluster. This cluster is set up in a high-availability configuration with both nodes active. Failure of any service causes that service to immediately rollover to the other node. The basic services necessary for ILThermo are a Web server, a Java application server, and a database. The ILThermo cluster currently uses Apache 2 as the Web server, Tomcat 5.5 as the java application server, and Oracle 10g as the database application. The first two elements, the Web server and application server, are deployed in a standard configuration. The database, on the publicly accessible ILThermo cluster, is a mirror of a highly secure NIST internal database. While steps have been taken to ensure the security of the database on the external server, this is not the primary data archive. A process is in place to

Table 1. Properties Included within the Present Scope of ILThermo

property group	property, units of display
Pure Ionic Liquids	
electrical conductivity	electrical conductivity, $S \cdot m^{-1}$
heat capacity and derived properties	heat capacity at constant pressure, $J \cdot K^{-1} \cdot mol^{-1}$
	heat capacity at vapor saturation pressure, $J \cdot K^{-1} \cdot mol^{-1}$
	standard enthalpy $H(T)-H(0)$, $kJ \cdot mol^{-1}$
	enthalpy function $(H(T)-H(0))/T$, $J \cdot K^{-1} \cdot mol^{-1}$
	standard entropy, $J \cdot K^{-1} \cdot mol^{-1}$
phase transition properties	enthalpy of transition or fusion, $kJ \cdot mol^{-1}$
	triple-point temperature, K
	glass transition temperature, K
	normal melting temperature, K
	solid−liquid equilibrium temperature, K
	solid−solid-phase transition temperature, K
refraction, surface tension, and speed of sound	surface tension, $N \cdot m^{-1}$
	refractive index (Na D-line), dimensionless
	speed of sound, $m \cdot s^{-1}$
transport properties	thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$
	thermal diffusivity, $m^2 \cdot s^{-1}$
	viscosity, Pa·s
vapor pressure and boiling temperature	phase boundary pressure, kPa
volumetric properties	specific density, $kg \cdot m^{-3}$
	molar volume, $m^3 \cdot mol^{-1}$
Binary Mixtures Involving Ionic Liquids	
activity, fugacity, and osmotic properties	activity coefficient at infinite dilution, dimensionless
composition at phase equilibrium	liquid−liquid equilibrium composition (various units)
	Henry's law constant for mole fraction, kPa
	solid−liquid equilibrium composition (various units)
	vapor−liquid−liquid equilibrium composition (various units)
	vapor−liquid equilibrium composition (various units)
	upper consolute composition (various units)
	eutectic composition (various units)
critical properties	upper consolute temperature, K
	critical temperature, K
	critical density, $kg \cdot m^{-3}$
	critical pressure, kPa
electrical conductivity	electrical conductivity, $S \cdot m^{-1}$
excess partial and apparent energetic properties	excess enthalpy (enthalpy of mixing), $kJ \cdot mol^{-1}$
	enthalpy of solution, $kJ \cdot mol^{-1}$
phase transition properties	eutectic temperature, K
	liquid−liquid equilibrium temperature, K
	solid−liquid equilibrium temperature, K
refraction, surface tension, and speed of sound	surface tension liquid−gas, $N \cdot m^{-1}$
	refractive index (Na D-line), dimensionless
	speed of sound, $m \cdot s^{-1}$
transport properties	binary diffusion coefficient, $10^{-9} \cdot m^2 \cdot s^{-1}$
	thermal diffusivity, $m^2 \cdot s^{-1}$
	viscosity, Pa·s
	kinematic viscosity, $m^2 \cdot s^{-1}$
vapor pressure, boiling temperature, and azeotropic temperature and pressure	phase boundary pressure, kPa
volumetric properties	specific density, $kg \cdot m^{-3}$
	excess volume, $m^3 \cdot mol^{-1}$
	molar volume, $m^3 \cdot mol^{-1}$
Ternary Mixtures Involving Ionic Liquids	
activity, fugacity, and osmotic properties	activity coefficient at infinite dilution, dimensionless
composition at phase equilibrium	distribution ratio, dimensionless
	liquid−liquid equilibrium composition (various units)
	tie-line data (various units)
	vapor−liquid equilibrium composition (various units)
critical properties	critical temperature, K
	critical density, $kg \cdot m^{-3}$
	critical pressure, kPa
electrical conductivity	electrical conductivity, $S \cdot m^{-1}$
excess partial and apparent energetic properties	enthalpy of solution, $kJ \cdot mol^{-1}$
phase transition properties	liquid−liquid equilibrium temperature, K
refraction, surface tension, and speed of sound	refractive index (Na D-line), dimensionless
refraction, surface tension, and speed of sound	speed of sound, $m \cdot s^{-1}$
transport properties	tracer diffusion coefficient, $10^{-9} \cdot m^2 \cdot s^{-1}$
	viscosity, Pa·s
vapor pressure, boiling temperature, and azeotropic temperature and pressure	phase boundary pressure, kPa
volumetric properties	specific density, $kg \cdot m^{-3}$
	molar volume, $m^3 \cdot mol^{-1}$

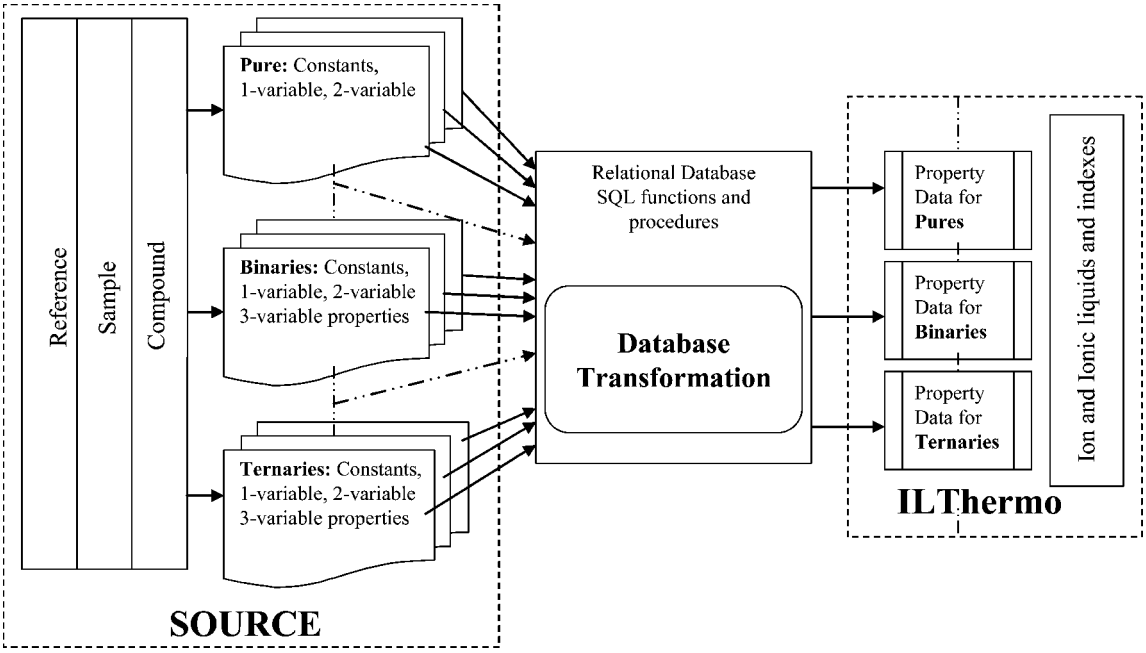


Figure 3. Illustration of the database transformation process.

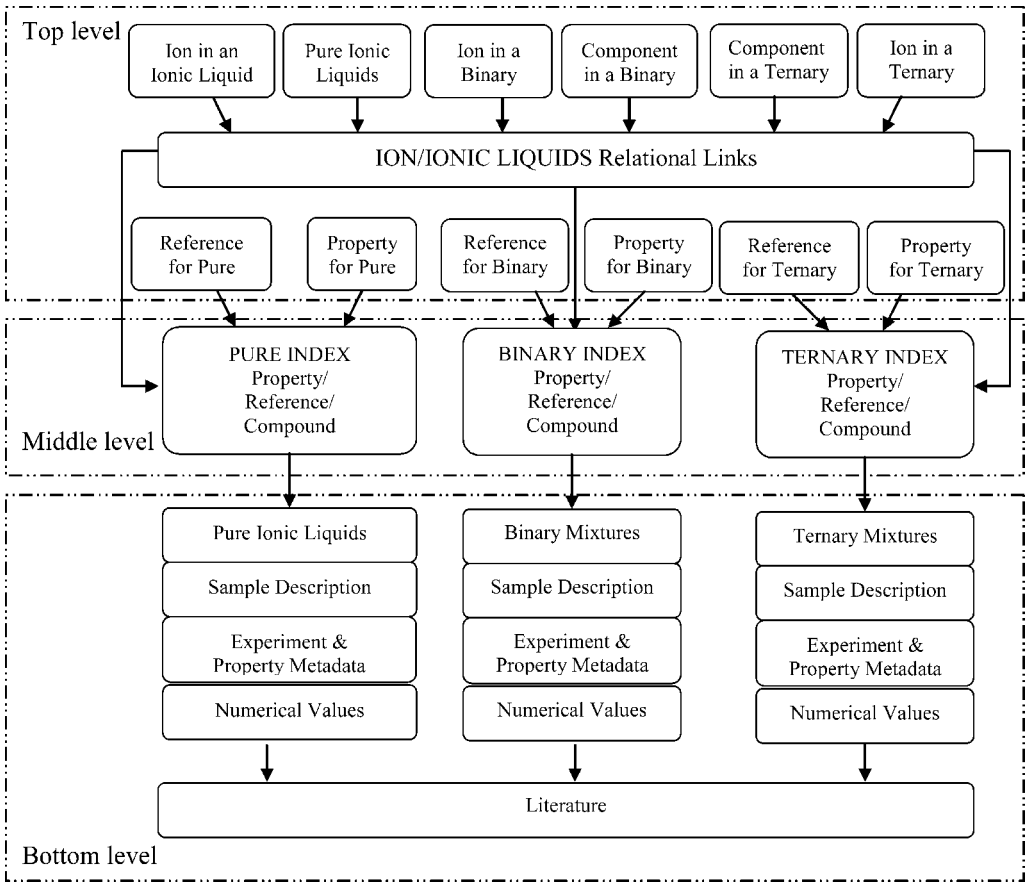


Figure 4. Database organization for ILThermo.

synchronize the external database with the primary internal database. However, this process never involves a direct connection of the primary, secure database to the public database on the external server, thus ensuring the integrity of the primary data.

Presentation Database Design. From a database design point of view, SOURCE is not intended for direct access to the end users, due to the complexity of its data structure. In managing complex physicochemical properties and chemical systems stored in the data system, SOURCE employs complicated specifications and a large number of database keys, codes, and conventions for identifying information in the database. Therefore, a lightweight presentation (read-only) database extracted from SOURCE, containing only the property data for ionic liquids, was developed for supporting Web data searches and presentation.

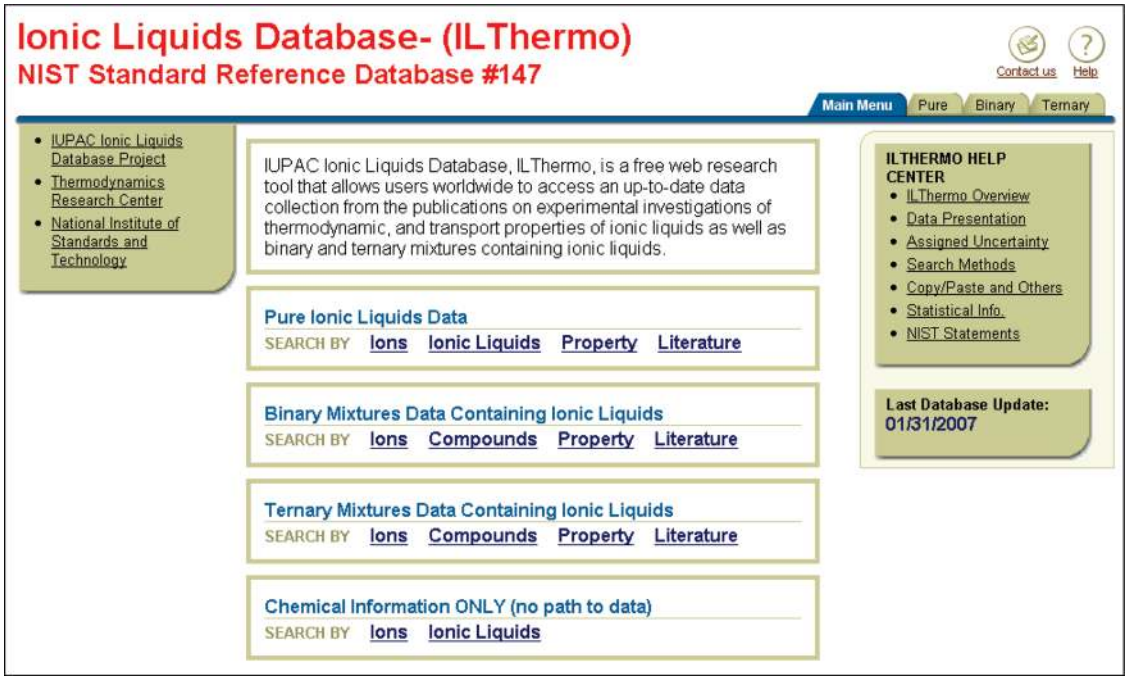


Figure 5. ILThermo main menu screen.

The ILThermo presentation database is the first database derived from SOURCE, with the data for ionic liquids representing a small subset of the extensive data in SOURCE. To create ILThermo, various data transformations were carried out with a set of database programming means, such as database views, functions, procedures, and packages written in Oracle PL/SQL, a procedural SQL language. Some typical tasks included (1) integration of relevant data and metadata information, (2) interpretation of information on chemical systems, properties, state variables, phases, and constraints, (3) restoration of significant digits of numerical values for presentation, (4) stripping out unwanted fields, and (5) adding new fields for convenient data presentation. A conceptual picture of the data transformation process is illustrated in Figure 3.

To fully present a specific measurement result, ILThermo contains six basic types of database records: (1) literature; (2) ion/compound; (3) sample; (4) measurement metadata, including full property specification and experimental method; (5) numerical values of property, variable, and uncertainty; and (6) relational links. In addition, it was important that the ILThermo presentation database generate a set of data indices to assist a high-performance search of ionic liquids and their mixtures. The data indices were created to enable a full search capacity for a particular task, such as searching property data by ion, ionic liquid, literature source, or property.

Another feature that distinguishes ILThermo from SOURCE lies in how the database is organized. Experimental information in SOURCE is organized with a strict hierarchy, starting from the literature and compound, followed by sample, then linked to the measured properties of pure or multiple components. In contrast, information is arranged in ILThermo at three separate levels (Figure 4). The top level is the *data availability layer*; the middle level is the *index layer*; and the bottom level is the *data layer*. At every level, records are organized into a parallel structure for properties of pure components, binary mixtures, or ternaries. The *data layer* contains records of sample description, experimental metadata, and numerical values of property, variable, and uncertainty. The *index layer* provides sufficient compound, property, and literature indexes for accomplishing all the search functionalities. The *data availability layer* contains a number of pre-selected lists of available ions, ionic liquids, properties, or references, generated from property data sets to meet the following search requirements:

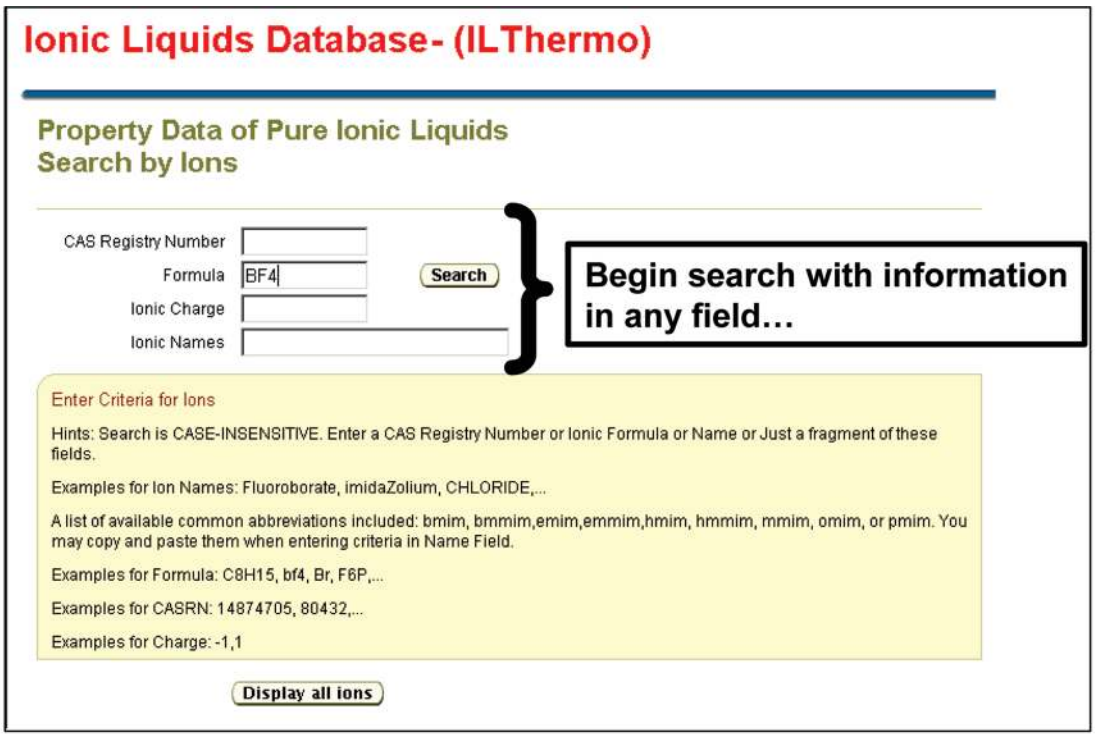
- Ions that are contained in pure ionic liquids with property data
- Ions that are contained in binary or ternary mixture systems with data
- Pure ionic liquids with data
- Ionic liquids contained in binary or ternary mixture systems with data
- Properties of pure ionic liquids or mixtures
- References of pure ionic liquids or mixtures

This organization of information permits flexible and parallel searches for the defined properties of pure components and mixtures.

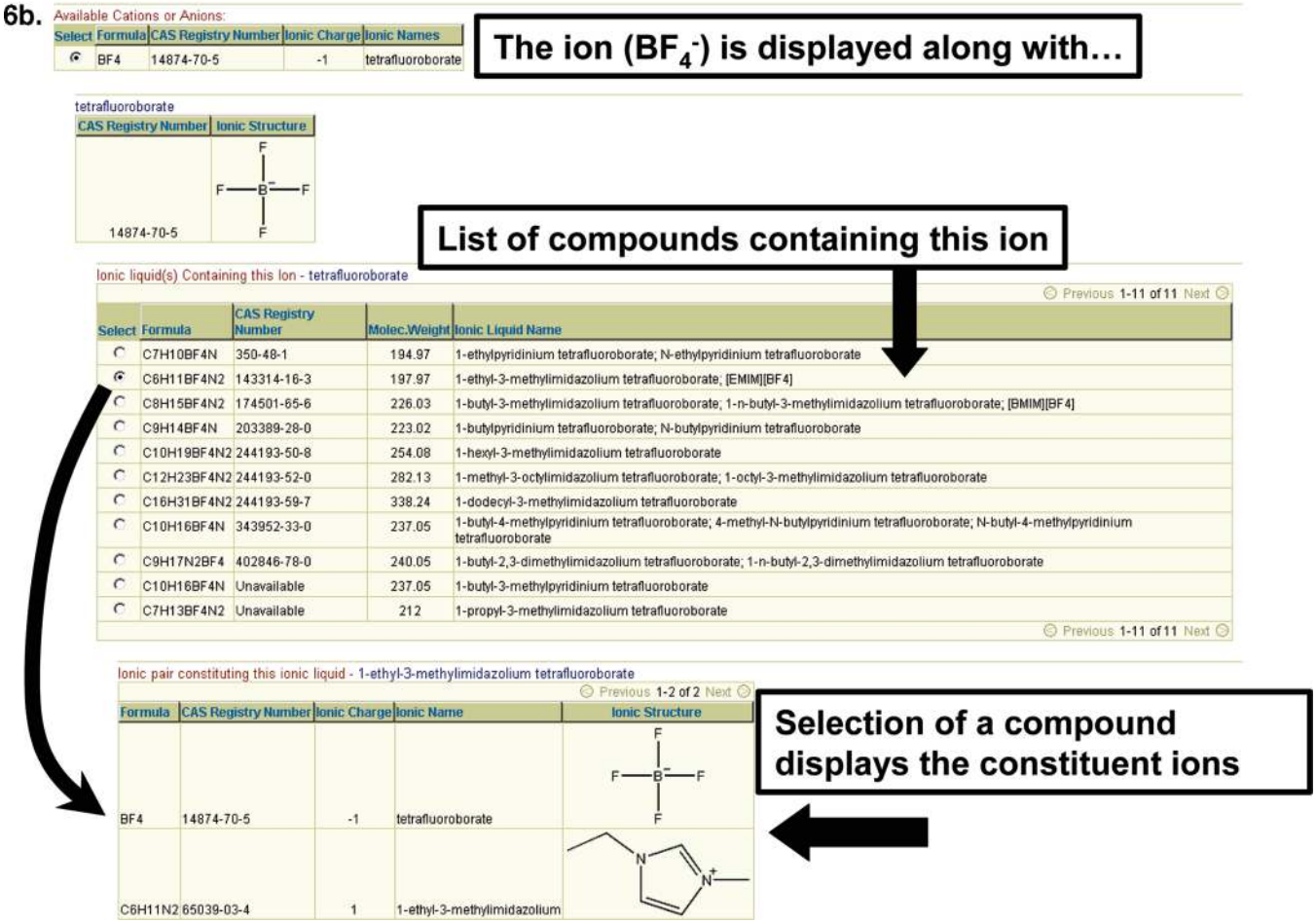
Ionic liquids are composed typically of organic cations with organic or inorganic anions, with most newer compounds consisting entirely of organic ions. Each ionic liquid and its constituent cation and anion has its own CASRN (Chemical Abstracts Service Registry Number), formula, and name synonyms. The ion specifications also include charge. Ions have no direct association with physicochemical properties. In accord with their ionic nature, structures for ionic liquids are presented to the user as representations of the separate ions. This data structure has the added benefit of allowing ready display in the database of all ionic liquids containing a common ion.

Web Publication Design. Many challenges exist in the development of Web-based applications. Such software has worldwide users, who may change quite dynamically. Due to the distributed, heterogeneous, and open nature of Web-based applications, complex multiserver, multicomputer, or multisoftware platforms are essential building components for their development and distribution. Moreover, the development of such software must often be accomplished within a short time[10] frame, yet still be of high quality. Thus, it is crucial to provide scalability, availability, and reliability for these applications and

6a.


Ionic Liquids Database- (ILThermo)
Property Data of Pure Ionic Liquids
Search by Ions
CAS Registry Number
Formula
BF4
Search
Ionic Charge
Ionic Names
Begin search with information in any field…
Enter Criteria for Ions
Hints: Search is CASE-INSENSITIVE. Enter a CAS Registry Number or Ionic Formula or Name or Just a fragment of these fields.
Examples for Ion Names: Fluoroborate, imidaZolium, CHLORIDE,...
A list of available common abbreviations included: bmim, bmmim,emim,emmim,hmim, hmmim, mmim, omim, or pmim. You may copy and paste them when entering criteria in Name Field.
Examples for Formula: C8H15, bf4, Br, F6P,...
Examples for CASRN: 14874705, 80432,...
Examples for Charge: -1,1
Display all ions

6b.


Available Cations or Anions:
Select | Formula | CAS Registry Number | Ionic Charge | Ionic Names
BF4 | 14874-70-5 | -1 | tetrafluoroborate
The ion (BF_4^-) is displayed along with…
tetrafluoroborate
CAS Registry Number | Ionic Structure
14874-70-5
List of compounds containing this ion
Ionic liquid(s) Containing this Ion - tetrafluoroborate
Previous 1-11 of 11 Next
Select | Formula | CAS Registry Number | Molec.Weight | Ionic Liquid Name
C7H10BF4N | 350-48-1 | 194.97 | 1-ethylpyridinium tetrafluoroborate; N-ethylpyridinium tetrafluoroborate
C6H11BF4N2 | 143314-16-3 | 197.97 | 1-ethyl-3-methylimidazolium tetrafluoroborate; [EMIM][BF4]
C8H15BF4N2 | 174501-65-6 | 226.03 | 1-butyl-3-methylimidazolium tetrafluoroborate; 1-n-butyl-3-methylimidazolium tetrafluoroborate; [BMIM][BF4]
C9H14BF4N | 203389-28-0 | 223.02 | 1-butylpyridinium tetrafluoroborate; N-butylpyridinium tetrafluoroborate
C10H19BF4N2 | 244193-50-8 | 254.08 | 1-hexyl-3-methylimidazolium tetrafluoroborate
C12H23BF4N2 | 244193-52-0 | 282.13 | 1-methyl-3-octylimidazolium tetrafluoroborate; 1-octyl-3-methylimidazolium tetrafluoroborate
C16H31BF4N2 | 244193-59-7 | 338.24 | 1-dodecyl-3-methylimidazolium tetrafluoroborate
C10H16BF4N | 343952-33-0 | 237.05 | 1-butyl-4-methylpyridinium tetrafluoroborate; 4-methyl-N-butylpyridinium tetrafluoroborate; N-butyl-4-methylpyridinium tetrafluoroborate
C9H17N2BF4 | 402846-78-0 | 240.05 | 1-butyl-2,3-dimethylimidazolium tetrafluoroborate; 1-n-butyl-2,3-dimethylimidazolium tetrafluoroborate
C10H16BF4N | Unavailable | 237.05 | 1-butyl-3-methylpyridinium tetrafluoroborate
C7H13BF4N2 | Unavailable | 212 | 1-propyl-3-methylimidazolium tetrafluoroborate
Previous 1-11 of 11 Next
Ionic pair constituting this ionic liquid - 1-ethyl-3-methylimidazolium tetrafluoroborate
Previous 1-2 of 2 Next
Formula | CAS Registry Number | Ionic Charge | Ionic Name | Ionic Structure
BF4 | 14874-70-5 | -1 | tetrafluoroborate
C6H11N2 | 65039-03-4 | 1 | 1-ethyl-3-methylimidazolium
Selection of a compound displays the constituent ions

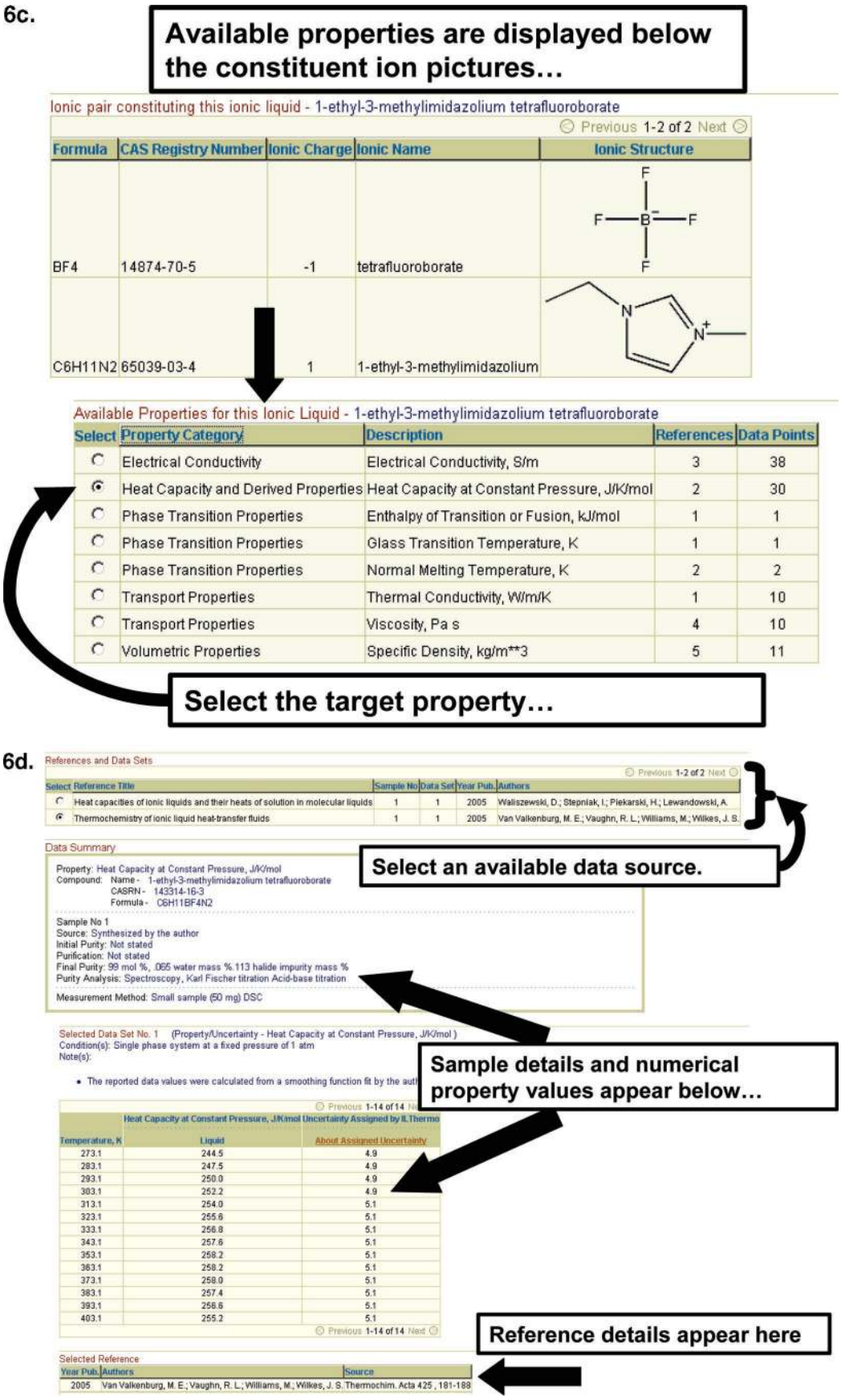


Figure 6. (a) Demonstration of ILThermo navigation: ion selection. (b) Demonstration of ILThermo navigation: compound selection and structure display. (c) Demonstration of ILThermo navigation: property selection. (d) Demonstration of ILThermo navigation: data source selection, sample display, numerical data display, and reference details.

essential to adopt well-designed frameworks and widely accepted modular design patterns in their development.

The Web presentation-oriented ILThermo was written in Java and utilizes the open, industry-standard J2EE platform[7] to develop an N-Tier, database-backed, and server-centric application. The decision for N-Tier application architecture[8] creates specific modular advantages that are vital to development efficiency and enhanced code maintenance. The entire ILThermo Web application is made up of five distinct tiers for handling the following functionality (Figure 2):

- Presentation database tier for ILThermo data storage and management
- Data model tier for object-relational data mapping (i.e., ILThermo tables and Java class objects)
- Application logic tier for search engine functionality including special Java codes for enhanced database searches
- Controller tier for handling user requests and responses and directing the data flow of a user session
- View tier for Web data presentation and user interactions

This design approach permits a clear separation of the core application logic from storage, presentation, and control logic, allowing different presentation views to share the same set of application data models, which aids rapid code development and maintenance.

Web Display of Ionic Liquids Data. ILThermo provides a variety of simple and robust search paths and tools to locate experimental property data for a specific ionic liquid or mixture. At the end of a search sequence, displayed numerical property data are those from a particular data set, for a particular property, within a particular literature source. Consequently, although it is possible to locate, for example, all literature sources containing measured densities for a particular ionic liquid, it is possible to display data from only a single source at one time. Data from different literature sources can be displayed sequentially.

The user interfaces consist primarily of main menu and submenu tabs, user entry forms for inputting search criteria, and the navigation elements needed to execute searches. The ILThermo main menu page (Figure 5) is the first page reached by the user upon visiting the database site. It provides the user with a single point of access to the database and is organized into four groups: (1) data for pure compounds, (2) data for binary mixtures, (3) data for ternary mixtures, and (4) chemical identification information only (formula, CASRN, structure, and ion charges) with no links to data.

Navigation from the main menu to any particular data set is achieved through Master/Detail data views in a hierarchical structure. A selection made in any displayed table results in an update of all content below that table. A "master" table is the upper table in a series, while a "detail" table is the table below. When an entry in the master table is selected, all available data pertinent to this entry will be populated in the sequential detail tables. Access to a particular data set can be initiated through any of the four choices (ion, compound, property, or literature) associated with the pure, binary mixture, or ternary mixture "Search By" boxes on the main menu (Figure 5). The term "compound" is used because it is possible to search, for example, for all mixtures involving an ionic liquid and water.

Typical navigation of ILThermo is demonstrated with a simple example (Figures 6a−d). In this example, the target data are heat capacities for 1-ethyl-3-methylimidazolium tetrafluoroborate ([EMIM][BF4]). The Ion link was used here, but in practice, the target data could be reached readily through the Ions, Ionic Liquid, or Property links. With this technology, ILThermo enables users to efficiently retrieve ionic liquid data within one page (after leaving the first search page) by navigating through a series of lists and tables.

All values of uncertainty are the combined expanded uncertainty with a level of confidence of 95 % estimated as part of the Ionic Liquids Database project (IUPAC Project 2003-020-2-100). Information provided by the authors in the text of the articles is considered in the uncertainty evaluation process. Numerous issues with regard to synthesis, purification, analysis, and measurement details for these materials often make estimation of uncertainties impossible without numerous assumptions. The listed values of the uncertainties should be considered preliminary and are subject to change as more information becomes available and analysis of the experimental data continues. Incorporation of the combined expanded uncertainties assessed on the basis of the Guide to the Expression of Uncertainty in Measurement ("the GUM")[9] was recommended by the IUPAC Task Group for the project *Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems* (IUPAC Project 2002-005-1-100). Terminology related to specification of uncertainties is as defined in GUM.[9] These ISO recommendations were adopted with minor editorial changes as the U.S. Guide to the Expression of Uncertainty in Measurement.[10] Applications of the GUM recommendations specifically for thermophysical and thermochemical property data have been discussed.[11]

Data Collection, Updates, Statistics, and Usage

Data collection for ILThermo is accomplished as part of the data-capture activities within the Thermodynamics Research Center (TRC) Data Entry Facility of NIST. Guided Data Capture (GDC) software[6] is used for structured capture of the data. Enhancements were made to GDC to allow full sample characterization of ionic liquids, including water and halide contents, and as many as four numerical purity values based on various analytical methods. The GDC software is available for free download from the Web (http://www.trc.nist.gov/GDC.html). Authors reporting experimental thermodynamic and thermophysical property data for ionic liquids and their mixtures are encouraged to contact the database managers at NIST (email: ILThermo@boulder.nist.gov) concerning inclusion of their work in the collection. The long-term success of the database project is dependent on the active participation of the user community.

Data in the ILThermo database are updated and revised (where necessary) approximately quarterly. Statistical information is maintained on the Web site for public access. As of January 2007, ILThermo contains information for a total of 204 ions and 321 ionic liquids. Among them, 114 pure ionic liquids have thermophysical property data with 7653 data points reported; 1000 binary mixtures with approximately 18 000 numerical property values; and 150 ternary systems with roughly 3500 numerical property values. The total number of experimental property values is near 30 000. It is important to note that these are all direct experimental values and that no derived values are included, such as excess volumes from densities or activity coefficients from vapor−liquid equilibrium studies.

ILThermo was released via a NIST public Web site in August of 2006 (http://ILThermo.boulder.nist.gov). Since its release, ILThermo usage has increased steadily. While the majority of usage is from U.S. government and commercial sites, there is also significant usage (approximately 30 %) from Europe, Japan, Russia, and other countries. This broad interest reflects the overall interest in ionic liquids in both research and commercial process development.

Summary

1. ILThermo is a new Web-based, open access, comprehensive source of thermophysical property data for pure ionic liquids, as well as for binary and ternary chemical systems in which an ionic liquid is a component.

2. The database is made available to users via the Web-Oracle data dissemination infrastructure recently established at NIST.

3. The mechanism of ILThermo deployment allows for frequent updates generated from the NIST TRC SOURCE Data Archival System.

4. Each numerical property value in ILThermo is characterized with an estimated combined expanded uncertainty, which is the most comprehensive measure of data quality.

5. Free access to ILThermo is available through the following URL: http://ILThermo.boulder.nist.gov/ILThermo/.

6. Authors reporting thermophysical property data for ionic liquids and their mixtures are encouraged to contact the ILThermo database managers at NIST (email: ILThermo@boulder.nist.gov) concerning inclusion of their work in the collection.

Acknowledgment

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