ILThermo: A Web Accessible Research Tool for Ionic Liquids

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20th International CODATA Conference

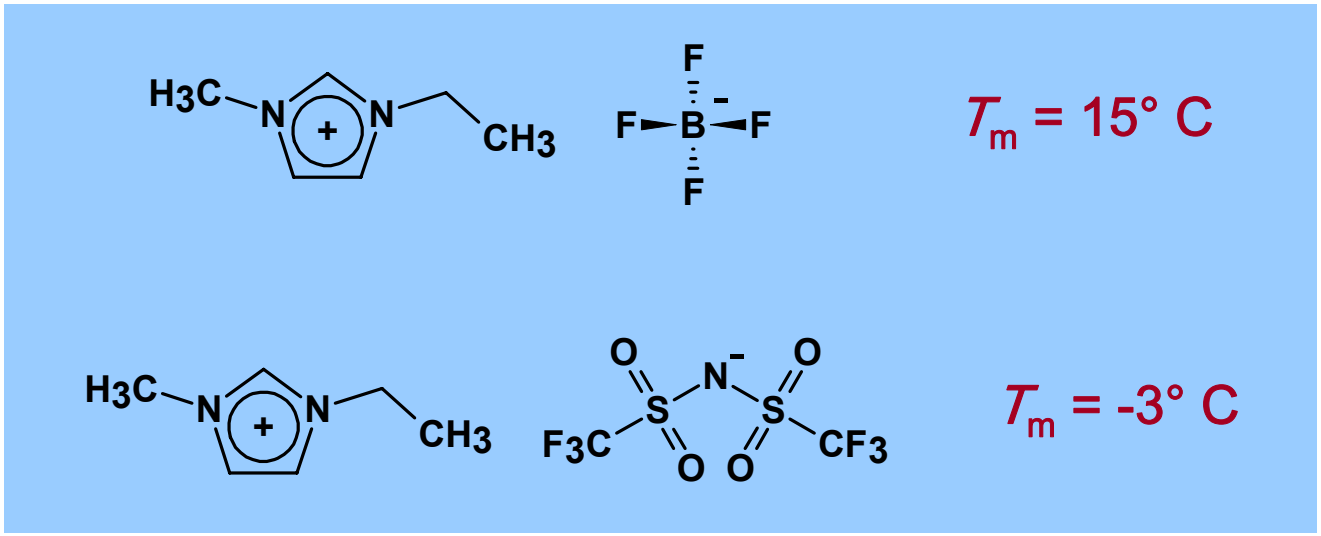
China Resources Hotel

Beijing, China

October 23-25, 2006

Ionic Liquids (ILs)

Ionic Liquids (ILs) are salts that melt at ≤ 100°C



- Non volatile - low vapor pressure
- Thermal stability
- Soluble in polar organic solvents
- Wide liquid range
- Electrochemical stability
- Non flammable
- Electrolytic conductivity

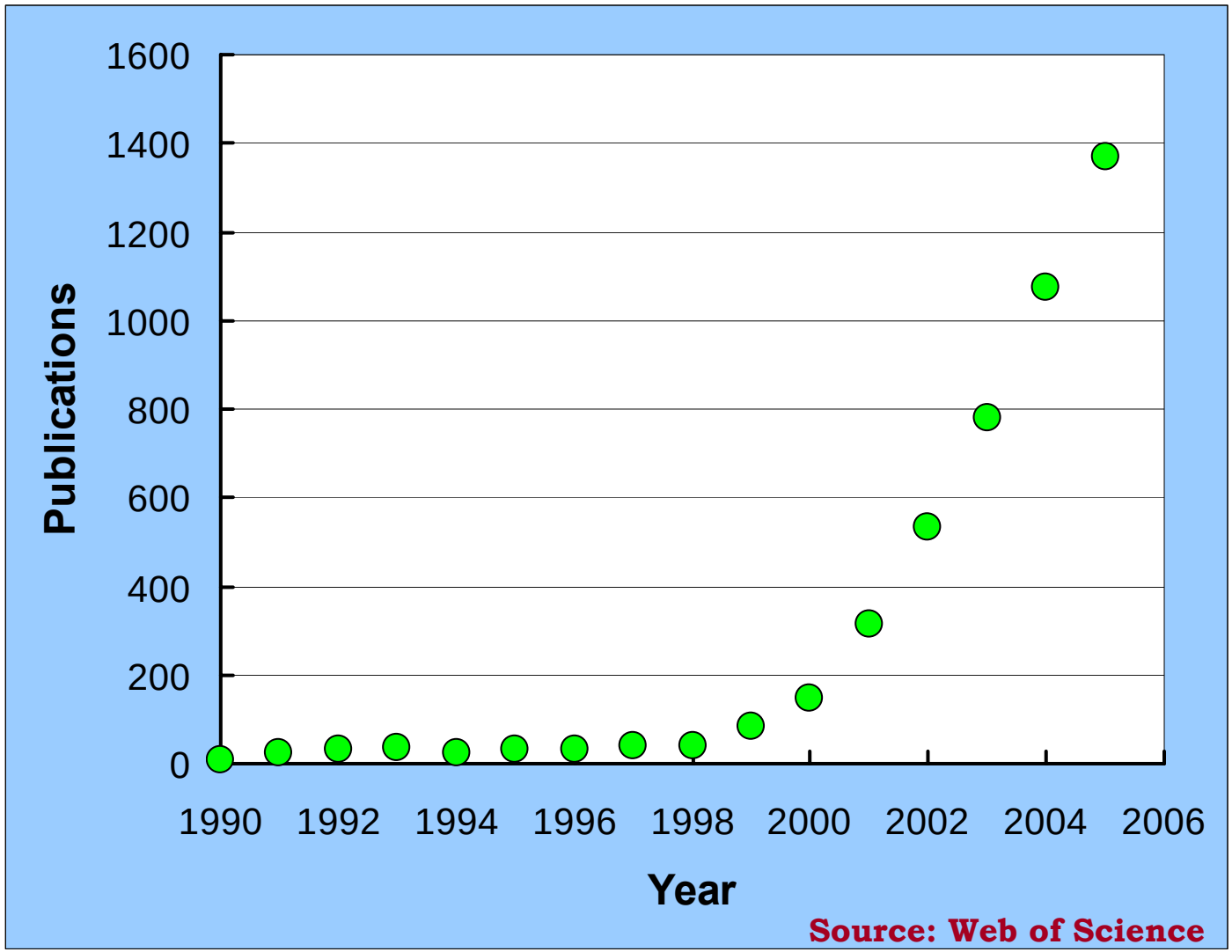
IL Applications

Low vapor pressure	→	Electrochemistry (batteries, electroplating)
Electrolytic conductivity	→	Separations (extraction, gas separation)
Electrochemical stability	→	Replacement for volatile solvents
Wide liquid range	→	Engineering liquids (lubricants, heat transfer fluids)
Good solvent properties		

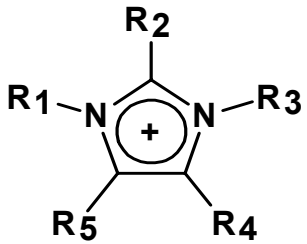
…and many others!

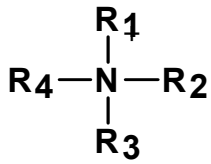
Need for a Database

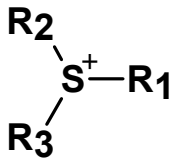
Dramatic increase in number of publications on the subject of ILs

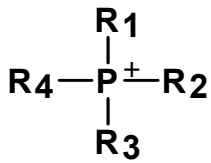


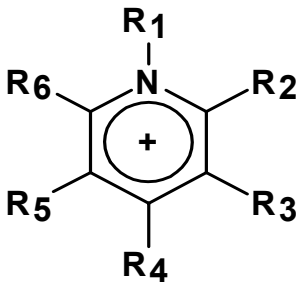
Need for a Database (Cont'd)

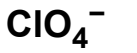


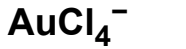


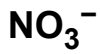


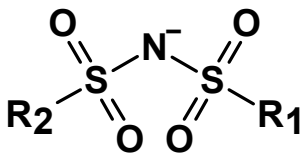


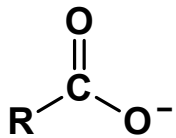


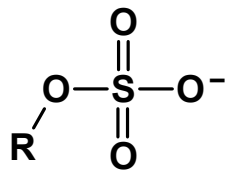










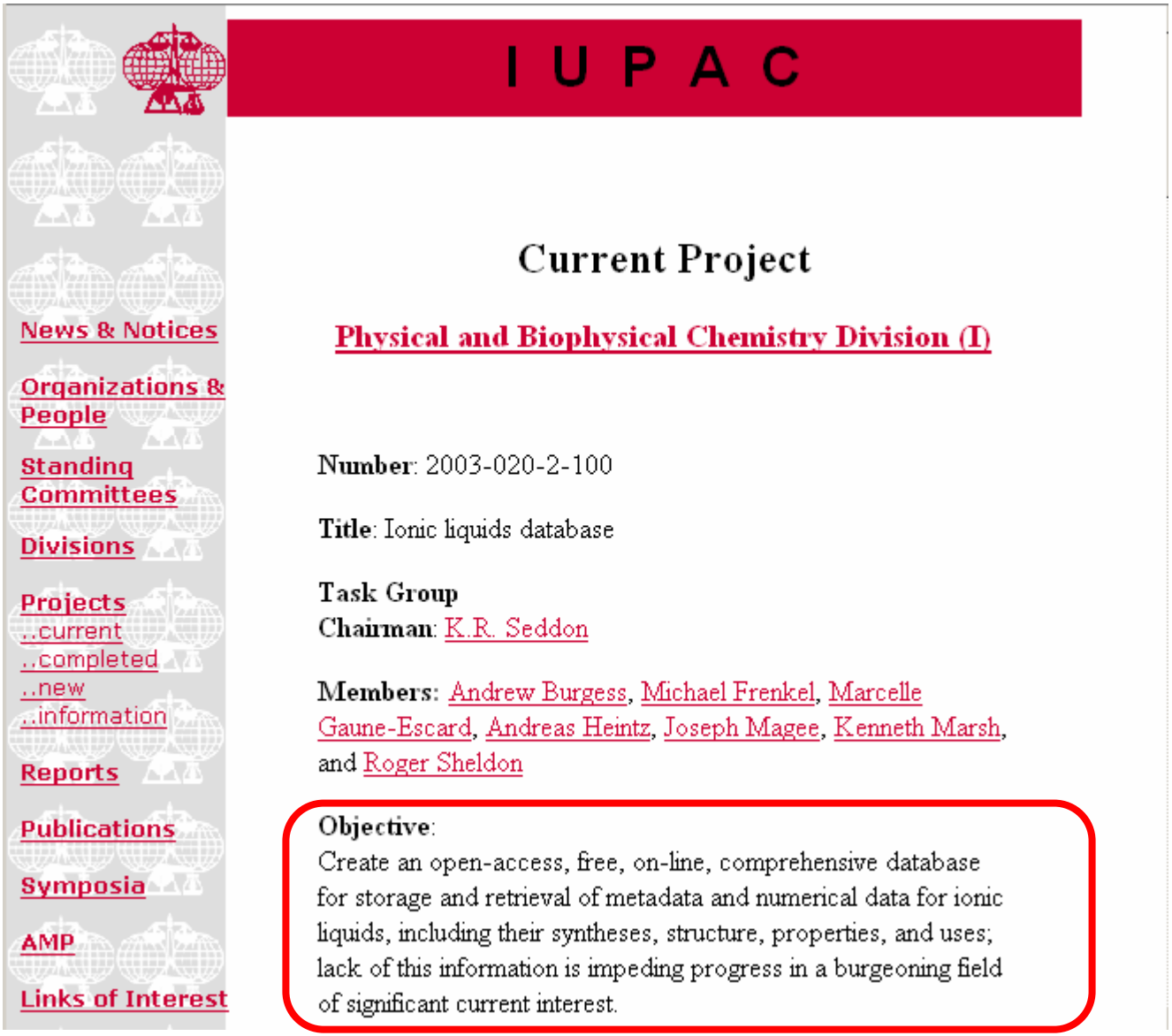


R = −H, $-CH_3$, $-CH_2CH_3$, $-CH_2CH_2CH_3$, $-(CH_2)_nCH_3$, $-CH(CH_3)_2$, $-CH_2OCH_3$ ....

Many combinations (different ILs) possible…
Perhaps as many as 10^{18} …
(Rogers, R. D.; Seddon, K. R. Science, 2003, 302, 792)

IUPAC Ionic Liquids Database Project

http://www.iupac.org/projects/2003/2003-020-2-100.html



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Current Project

Physical and Biophysical Chemistry Division (I)

Number: 2003-020-2-100

Title: Ionic liquids database

Task Group
Chairman: K.R. Seddon

Members: Andrew Burgess, Michael Frenkel, Marcelle Gaune-Escard, Andreas Heintz, Joseph Magee, Kenneth Marsh, and Roger Sheldon

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.

1st Task Group Meeting

Delft University of Technology
Delft, Netherlands January 26, 2004

- Present: Andrew Burgess, Marcelle Gaune-Escard, Michael Frenkel, Joseph Magee, Kenneth Marsh, Kenneth Seddon, Roger Sheldon (host), Sergey Verevkin (for Andreas Heintz)
- A distributed access database would be developed with various types of data being independently managed
- Coverage would include synthesis, catalysis, structure, manufacturing, modeling as well as physical and chemical property data
- New required fields in the primary database were defined including those for handling polymers and enzymes
- Ensuring complementarity with high-temperature molten salt data and the QUILL database, avoiding duplication of effort

Minutes of First Ionic Liquids Database Meeting
(#2003-020-2-100)
Delft University of Technology, 26th January 2004

Present: Andrew Burgess, Marcelle Gaune-Escard, Michael Frenkel, Joseph W. Magee, Kenneth N. Marsh, Kenneth Richard Seddon, Roger Sheldon, Sergey P. Verevkin (standing in for Andreas Heintz)

Opening Remarks

The Committee expressed their thanks to Prof. Sheldon for hosting the meeting.

NIST Database Projects

Drs. Magee and Frenkel gave a detailed presentation on the structure and input methods for extant NIST databases. In particular, the relationship between the primary NIST thermodynamic database and the new ionic liquid database was explored; the product should be exportable to Aspen. The importance of the ionic liquid workshop at the 17th IUPAC Conference on Chemical Thermodynamics in Rostock, Germany, 28th July to 2nd August, 2002 in defining the current project was noted. The slides are attached as an Appendix to this report.

Discussion

1. New Required Fields

The requirements of ionic materials, as compared with molecular systems, mean that new fields in the primary database need to be defined. The absolute minimum basic requirements are:

- Stoicheiometry of salt
- Name of anion
- CAS registry number of anion
- Name of cation
- CAS registry number of cation
- Electrical conductivity

Desirable extra fields would be:

- Lattice energy (both theoretical and "experimental")
- Dielectric constant (frequency dependent)
- Oxygen sensitivity (Boolean)
- Water sensitivity (Boolean)
- Corrosion data (text file)
- Solubility data (Boolean)
- Enzyme activation (Boolean)
- Items to be inserted into the QUILL structural and spectroscopic database:
- X-ray structural data
- Neutron structural data
- EXAFS structural data
- Spectroscopic data (MS, NMR, IR, Raman, *etc.*)
- Thermal data (TGA, DSC)
- Toxicity data

Images are most conveniently incorporated as jpeg files.

2nd Task Group Meeting

Beijing International Convention Center
Beijing, China August 12, 2005

- Present: Marcelle Gaune-Escard, Michael Frenkel, Joseph Magee, Kenneth Marsh, Kenneth Seddon, Slobodan Gadzuric (observer)
- Structure and information input methods for ILThermo
  - Guided Data Capture (GDC) software
  - ThermoML IUPAC standard for storage and exchange of data
- Search / retrieval from ILThermo
- Public release of ILThermo – will follow internal review procedures
- Distributed access system – a desirable long-range goal with various types of data being independently managed
- Coverage would include synthesis, catalysis, structure, manufacturing, modeling as well as physical and chemical property data with their associated uncertainties
- Avoid duplication of effort – populate ILThermo with high-temperature molten salt data and coordinate efforts with other database developers

MINUTES OF SECOND IONIC LIQUIDS DATABASE MEETING
(#2003-020-2-100)

IUPAC GENERAL ASSEMBLY
BEIJING INTERNATIONAL CONVENTION CENTER
BEIJING, CHINA, 12TH AUGUST 2005

PRESENT

Kenneth R. Seddon (Chair), Kenneth N. Marsh, Marcelle Gaune-Escard, Joseph W. Magee, Michael Frenkel (members) and Slobodan Gadzuric (observer)

OPENING REMARKS

The Chair welcomed all in attendance. Apologies were offered from those unable to attend. Introductions were made. The Task Group expressed their thanks to IUPAC-GA organizers for hosting the meeting and logistical support for the IL database task group meeting.

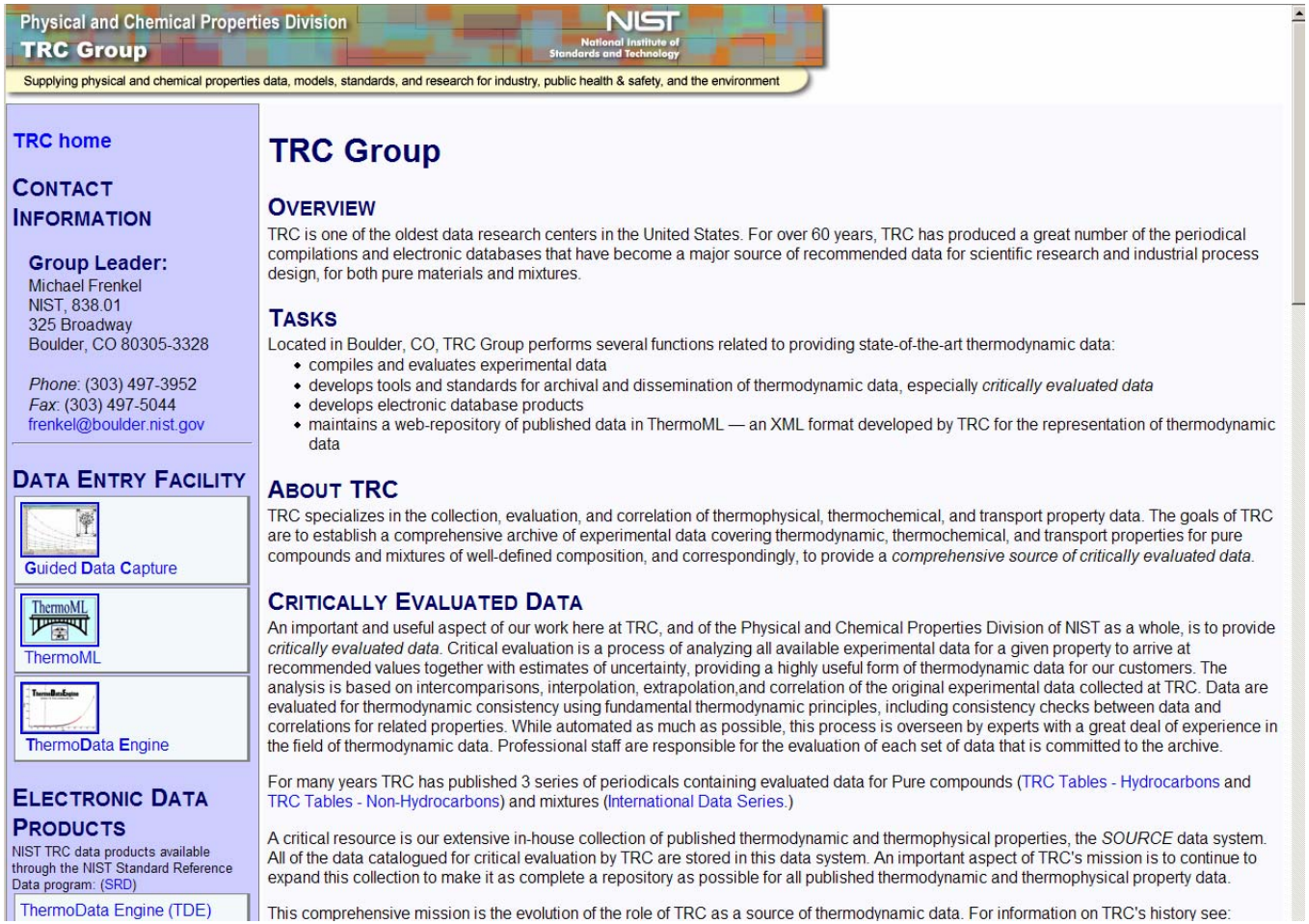
DATABASE PROJECT UPDATE

Drs. Magee and Frenkel of NIST gave a detailed presentation on the structure and input methods for the recently developed database, called ILThermo. The discussion began with a review of the background and genesis of the project, as follows. Progress in utilizing ionic liquids had been hampered by the lack of an open-access, public domain, comprehensive data retrieval system scoped to cover information pertaining to ionic liquids. Development of such a database infrastructure encompasses a number of complex issues related to data submission, processing, mining, quality control, management, critical evaluation, and dissemination. It is also obvious that such a system should provide coverage for various types of data such as synthesis, catalysis, structure, manufacturing, modeling as well as thermophysical and thermochemical property data. A broad-based international effort would be needed to develop such an information system. Thus the present IUPAC project (2003-020-2-100) *Ionic Liquids Database* (K. R. Seddon (Task Group Chair), A. Burgess, M. Frenkel, M. Gaune-Escard, A. Heintz, J. W. Magee, K. N. Marsh, R. Sheldon (members)) was formed to address this need.

On January 26, 2004 the task group met at the Technical University of Delft (Delft, Netherlands) to decide on a common vision for the project and to divide the data collection effort amongst the participants. A second meeting had been deemed necessary when a preliminary version of the database was ready for testing.

The discussion then turned to the preliminary version of the ionic liquids database and exploring future tasks. In particular, the relationship between the primary NIST molten salt database and the new ionic liquids database was explored. The enormous number of publications concerning ionic liquids in 2004 (approx. 2500 papers) and the foreseeable growth expected in the future requires proper data collection, storage and retrieval from searchable electronic archives. The new database will be significantly more inclusive than NIST Standard Reference Database 27: NIST Molten Salts Database that provides molten state properties (density, surface tension, viscosity, electrical conductance) for 320 inorganic salts and 4,000 mixtures.

IUPAC Ionic Liquids Database Development: Thermodynamics Research Center (TRC)



Physical and Chemical Properties Division
TRC Group
NIST National Institute of Standards and Technology
Supplying physical and chemical properties data, models, standards, and research for industry, public health & safety, and the environment

TRC home

CONTACT INFORMATION

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Boulder, CO 80305-3328

Phone: (303) 497-3952
Fax: (303) 497-5044
frenkel@boulder.nist.gov

DATA ENTRY FACILITY

Guided Data Capture

ThermoML

ThermoData Engine

ELECTRONIC DATA PRODUCTS

NIST TRC data products available through the NIST Standard Reference Data program: (SRD)

ThermoData Engine (TDE)

TRC Group

OVERVIEW

TRC is one of the oldest data research centers in the United States. For over 60 years, TRC has produced a great number of the periodical compilations and electronic databases that have become a major source of recommended data for scientific research and industrial process design, for both pure materials and mixtures.

TASKS

Located in Boulder, CO, TRC Group performs several functions related to providing state-of-the-art thermodynamic data:

- compiles and evaluates experimental data
- develops tools and standards for archival and dissemination of thermodynamic data, especially *critically evaluated data*
- develops electronic database products
- maintains a web-repository of published data in ThermoML — an XML format developed by TRC for the representation of thermodynamic data

ABOUT TRC

TRC specializes in the collection, evaluation, and correlation of thermophysical, thermochemical, and transport property data. The goals of TRC are to establish a comprehensive archive of experimental data covering thermodynamic, thermochemical, and transport properties for pure compounds and mixtures of well-defined composition, and correspondingly, to provide a *comprehensive source of critically evaluated data*.

CRITICALLY EVALUATED DATA

An important and useful aspect of our work here at TRC, and of the Physical and Chemical Properties Division of NIST as a whole, is to provide *critically evaluated data*. Critical evaluation is a process of analyzing all available experimental data for a given property to arrive at recommended values together with estimates of uncertainty, providing a highly useful form of thermodynamic data for our customers. The analysis is based on intercomparisons, interpolation, extrapolation,and correlation of the original experimental data collected at TRC. Data are evaluated for thermodynamic consistency using fundamental thermodynamic principles, including consistency checks between data and correlations for related properties. While automated as much as possible, this process is overseen by experts with a great deal of experience in the field of thermodynamic data. Professional staff are responsible for the evaluation of each set of data that is committed to the archive.

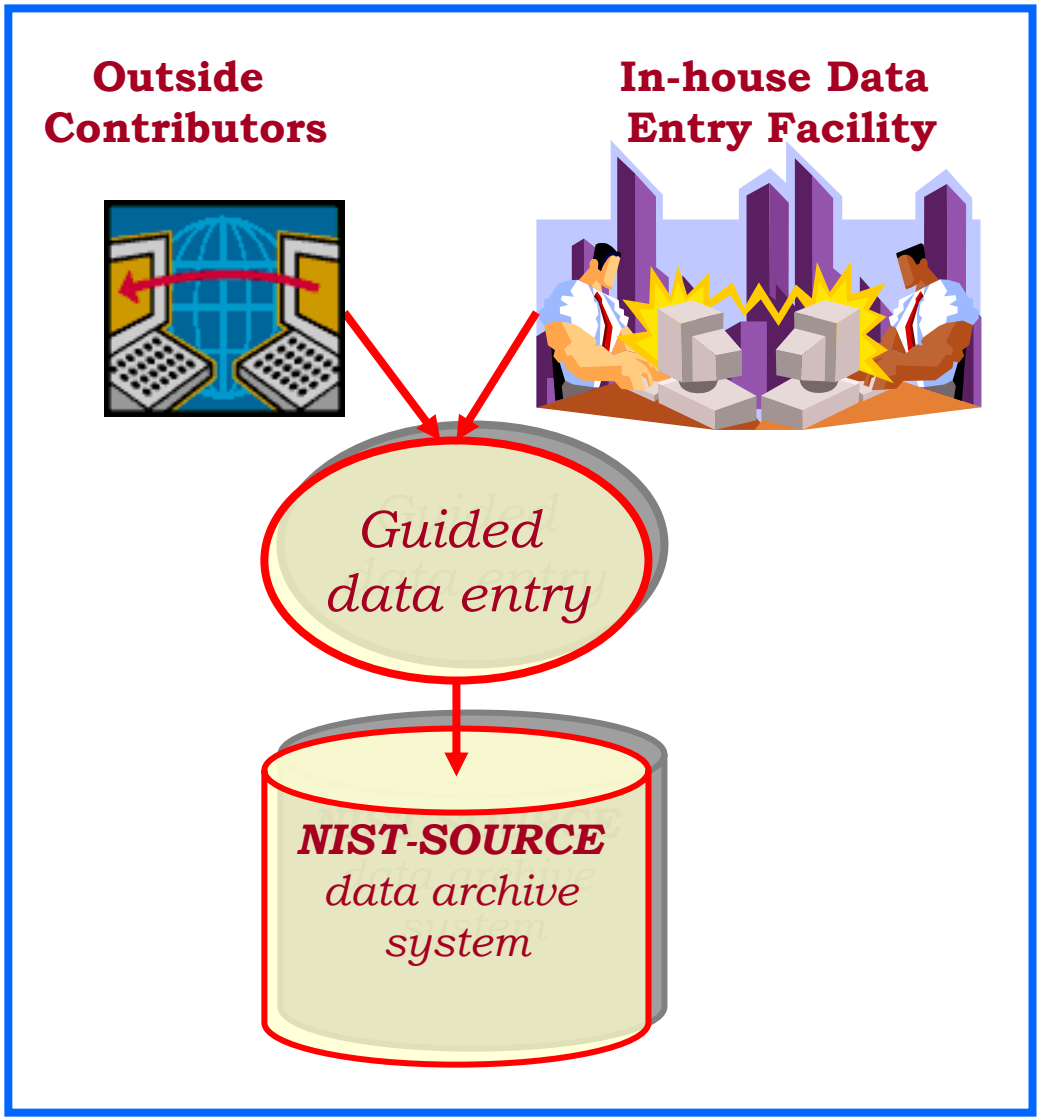
For many years TRC has published 3 series of periodicals containing evaluated data for Pure compounds (TRC Tables - Hydrocarbons and TRC Tables - Non-Hydrocarbons) and mixtures (International Data Series.)

A critical resource is our extensive in-house collection of published thermodynamic and thermophysical properties, the *SOURCE* data system. All of the data catalogued for critical evaluation by TRC are stored in this data system. An important aspect of TRC's mission is to continue to expand this collection to make it as complete a repository as possible for all published thermodynamic and thermophysical property data.

This comprehensive mission is the evolution of the role of TRC as a source of thermodynamic data. For information on TRC's history see:

http://trc.nist.gov/

NIST-SOURCE System for Data Capture and Storage



NIST-SOURCE

Depository of Over 150 experimental thermophysical and thermochemical properties reported in the world's scientific literature

Includes

✓*over 2,500,000 numerical property values and their uncertainties*

✓ *data entry rate is near 400,000 values per year*

NIST-SOURCE for ILs Data Capture and Storage

Outside Contributors

In-house Data Entry Facility

Guided data entry

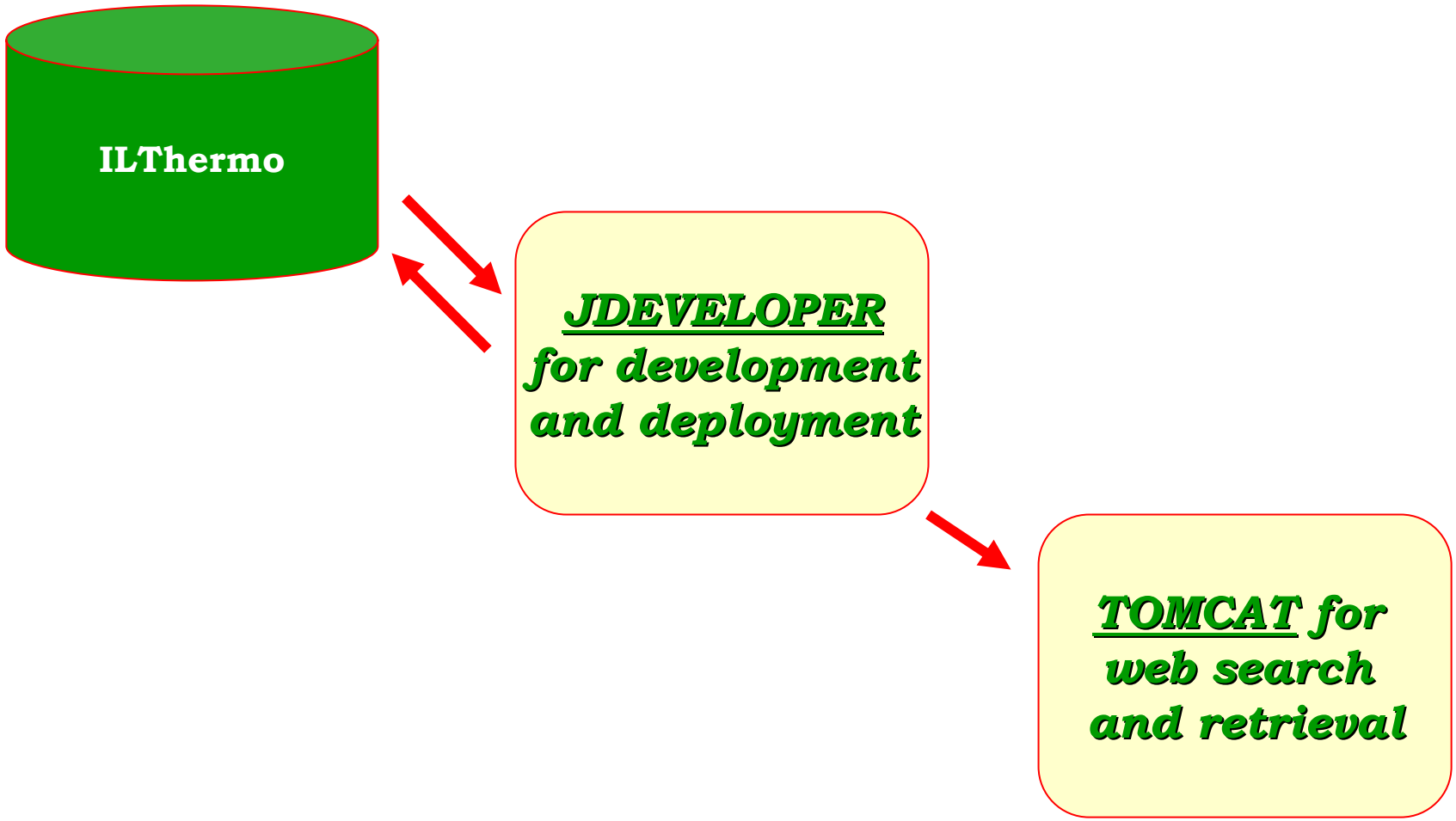
NIST-SOURCE *data archive system*

ILThermo (read-only DB)

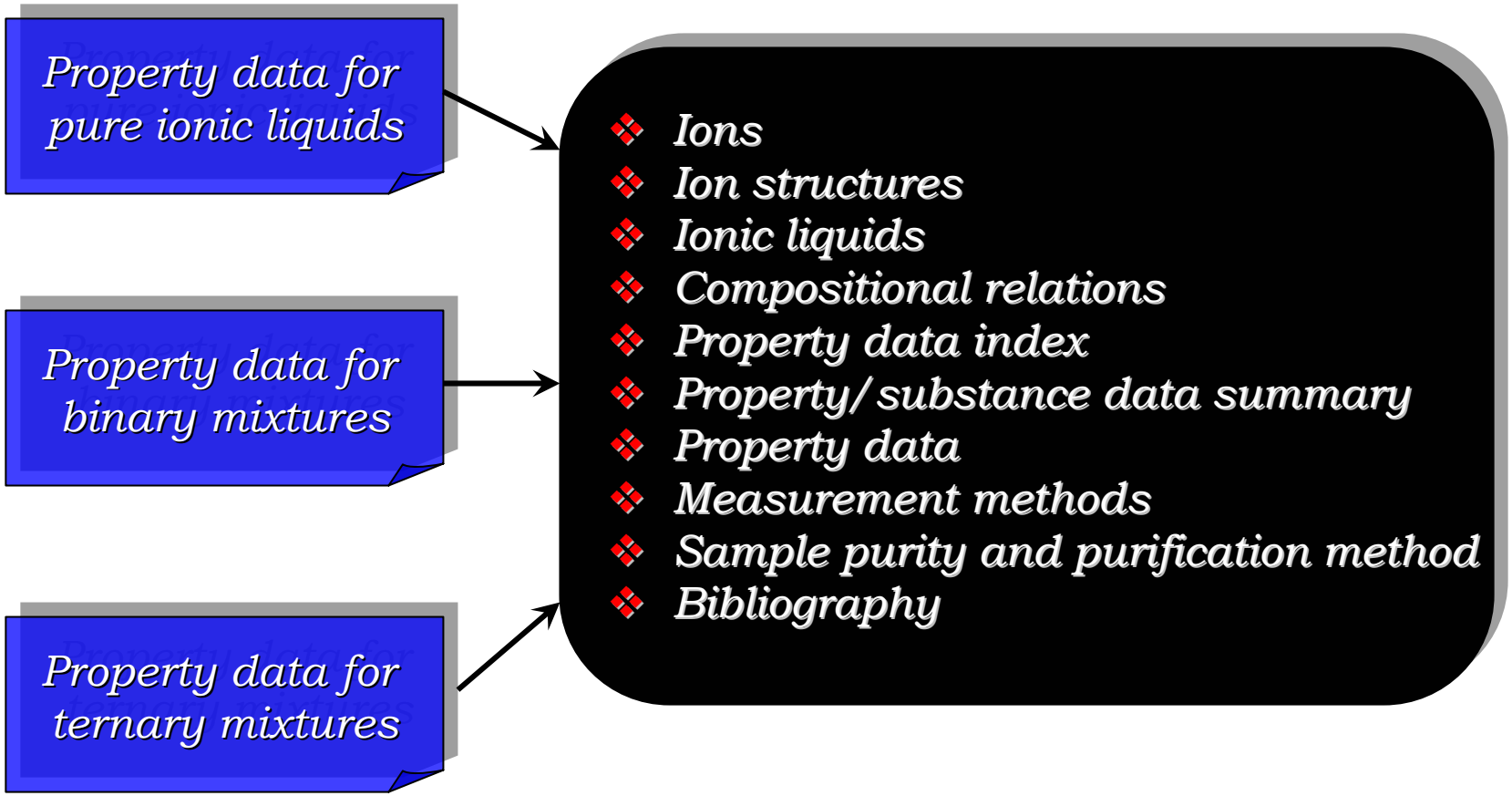
IL Data Retrieval System (Oracle PL/SQL)

… also the means for regular updates!

ILThemo – Interface and Web Deployment

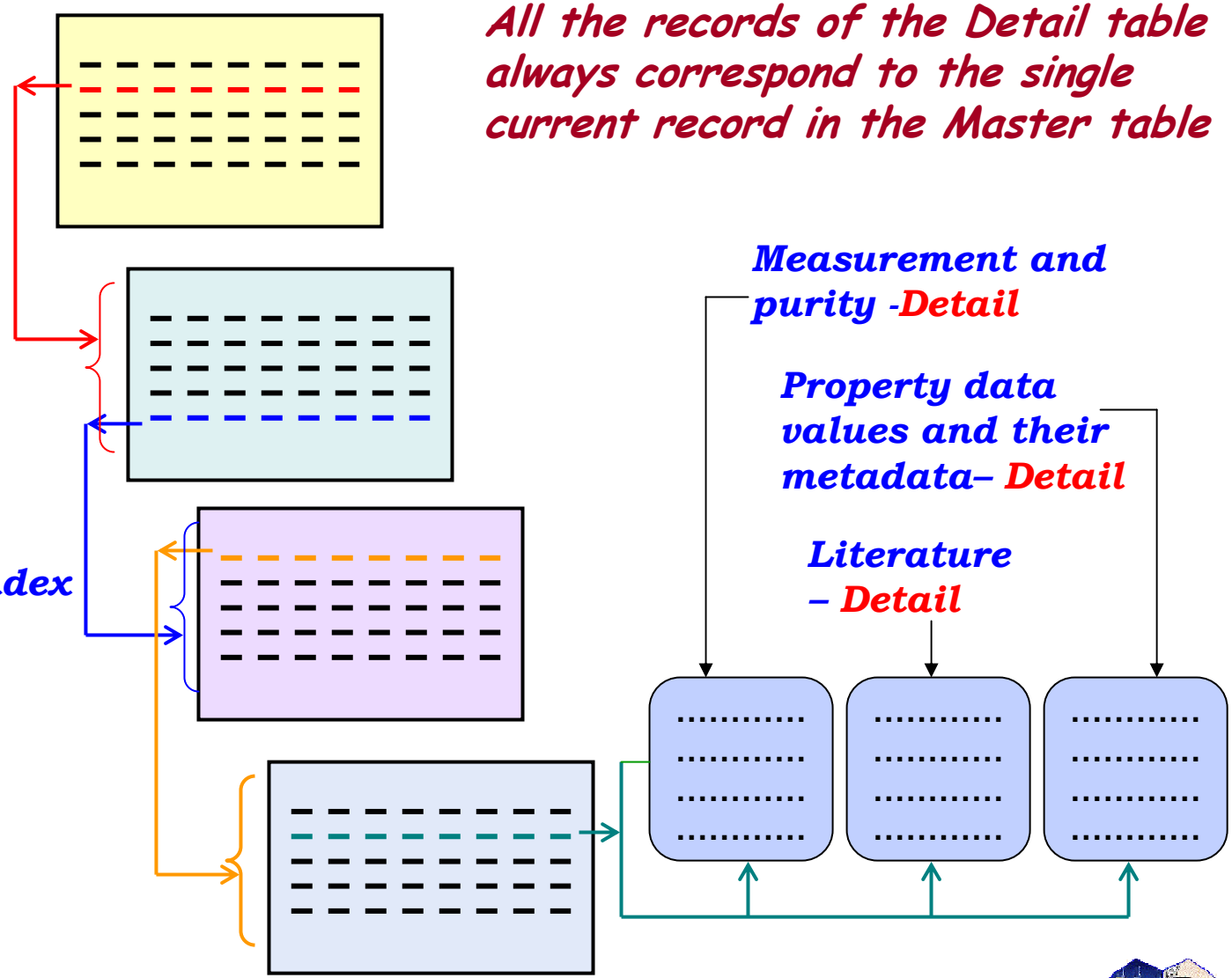


What's in *ILThermo*?



Data Presentation: Master/Detail Relationship

All the records of the Detail table always correspond to the single current record in the Master table

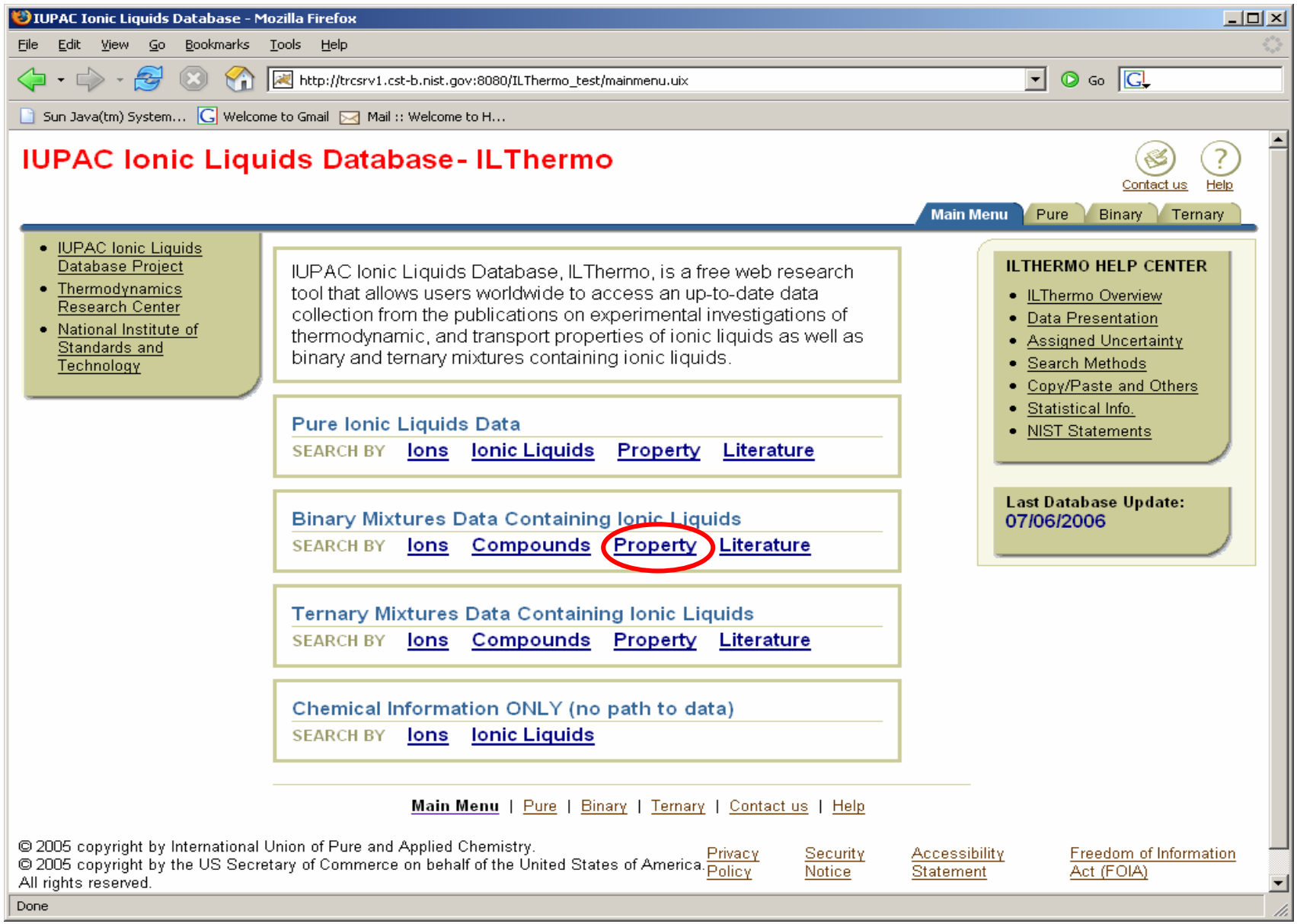


ILThermo

Public Release – 31 July 2006

http://ilthermo.boulder.nist.gov

How Do I Search for Information in *ILThermo*?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http://trcsrv1.cst-b.nist.gov:8080/ILThermo_test/mainmenu.uix
Go
Sun Java(tm) System...
Welcome to Gmail
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Main Menu
Pure
Binary
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IUPAC Ionic Liquids Database Project
Thermodynamics Research Center
National Institute of Standards and Technology
IUPAC Ionic Liquids Database, ILThermo, is a free web research tool that allows users worldwide to access an up-to-date data collection from the publications on experimental investigations of thermodynamic, and transport properties of ionic liquids as well as binary and ternary mixtures containing ionic liquids.
Pure Ionic Liquids Data
SEARCH BY Ions Ionic Liquids Property Literature
Binary Mixtures Data Containing Ionic Liquids
SEARCH BY Ions Compounds Property Literature
Ternary Mixtures Data Containing Ionic Liquids
SEARCH BY Ions Compounds Property Literature
Chemical Information ONLY (no path to data)
SEARCH BY Ions Ionic Liquids
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Data Presentation
Assigned Uncertainty
Search Methods
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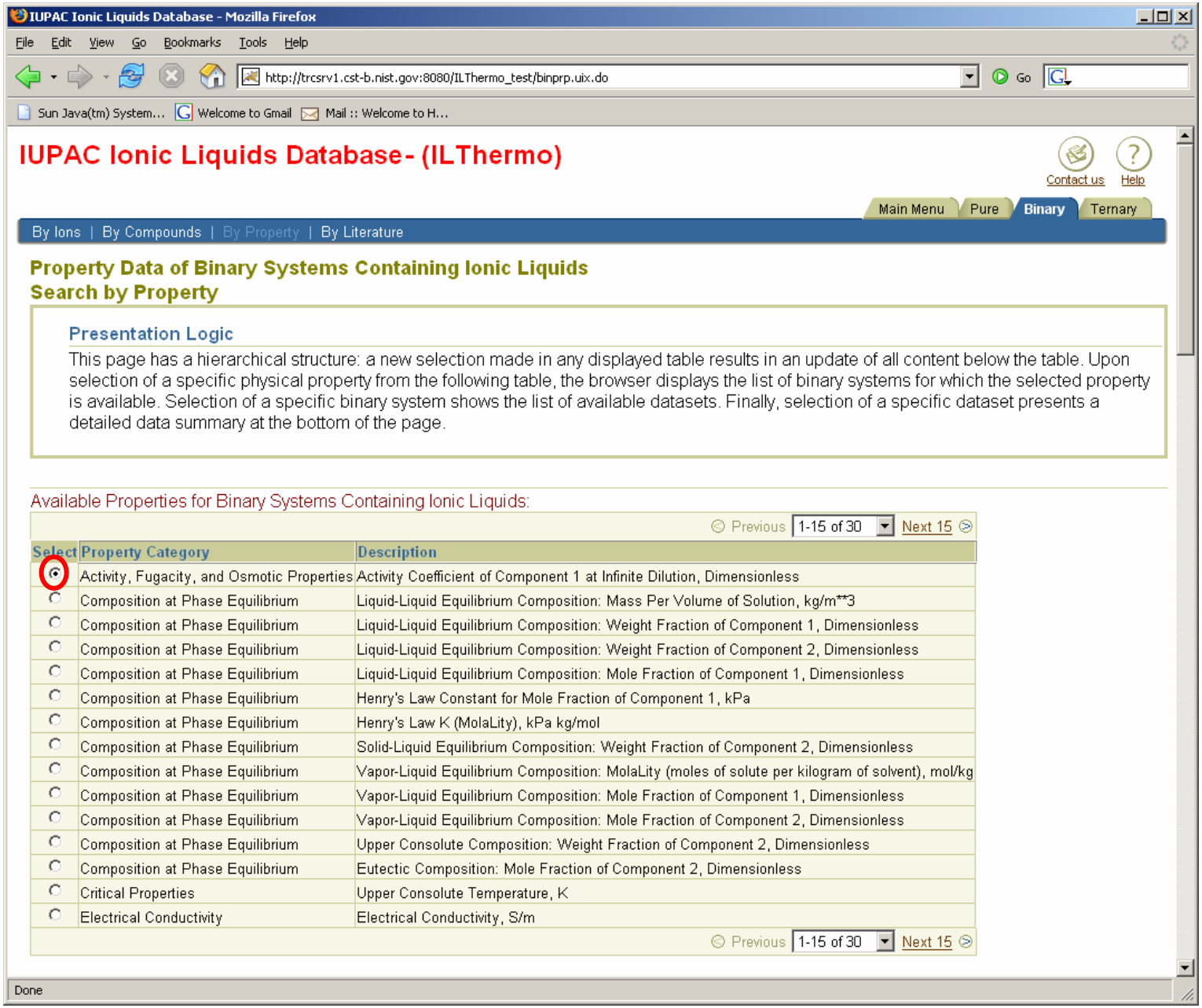
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http://trcsrv1.cst-b.nist.gov:8080/ILThermo_test/binprp.uix.do
Go
Sun Java(tm) System... Welcome to Gmail Mail :: Welcome to H...
IUPAC Ionic Liquids Database- (ILThermo)
Contact us
Help
Main Menu
Pure
Binary
Ternary
By Ions | By Compounds | By Property | By Literature
Property Data of Binary Systems Containing Ionic Liquids
Search by Property
Presentation Logic
This page has a hierarchical structure: a new selection made in any displayed table results in an update of all content below the table. Upon selection of a specific physical property from the following table, the browser displays the list of binary systems for which the selected property is available. Selection of a specific binary system shows the list of available datasets. Finally, selection of a specific dataset presents a detailed data summary at the bottom of the page.
Available Properties for Binary Systems Containing Ionic Liquids:
Previous 1-15 of 30 Next 15
Select
Property Category
Description
Activity, Fugacity, and Osmotic Properties
Activity Coefficient of Component 1 at Infinite Dilution, Dimensionless
Composition at Phase Equilibrium
Liquid-Liquid Equilibrium Composition: Mass Per Volume of Solution, kg/m**3
Composition at Phase Equilibrium
Liquid-Liquid Equilibrium Composition: Weight Fraction of Component 1, Dimensionless
Composition at Phase Equilibrium
Liquid-Liquid Equilibrium Composition: Weight Fraction of Component 2, Dimensionless
Composition at Phase Equilibrium
Liquid-Liquid Equilibrium Composition: Mole Fraction of Component 1, Dimensionless
Composition at Phase Equilibrium
Henry's Law Constant for Mole Fraction of Component 1, kPa
Composition at Phase Equilibrium
Henry's Law K (MolaLity), kPa kg/mol
Composition at Phase Equilibrium
Solid-Liquid Equilibrium Composition: Weight Fraction of Component 2, Dimensionless
Composition at Phase Equilibrium
Vapor-Liquid Equilibrium Composition: MolaLity (moles of solute per kilogram of solvent), mol/kg
Composition at Phase Equilibrium
Vapor-Liquid Equilibrium Composition: Mole Fraction of Component 1, Dimensionless
Composition at Phase Equilibrium
Vapor-Liquid Equilibrium Composition: Mole Fraction of Component 2, Dimensionless
Composition at Phase Equilibrium
Upper Consolute Composition: Weight Fraction of Component 2, Dimensionless
Composition at Phase Equilibrium
Eutectic Composition: Mole Fraction of Component 2, Dimensionless
Critical Properties
Upper Consolute Temperature, K
Electrical Conductivity
Electrical Conductivity, S/m
Previous 1-15 of 30 Next 15
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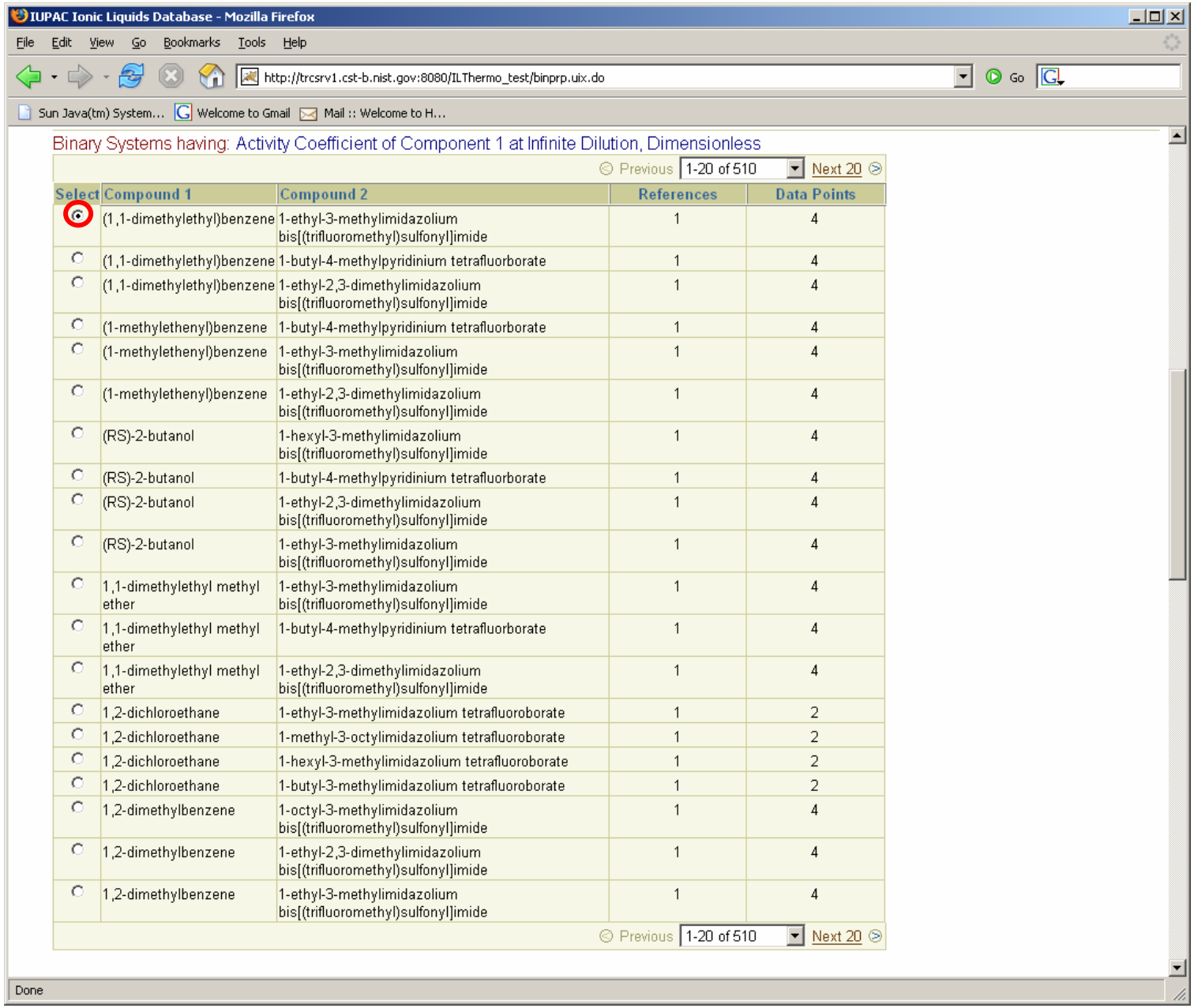
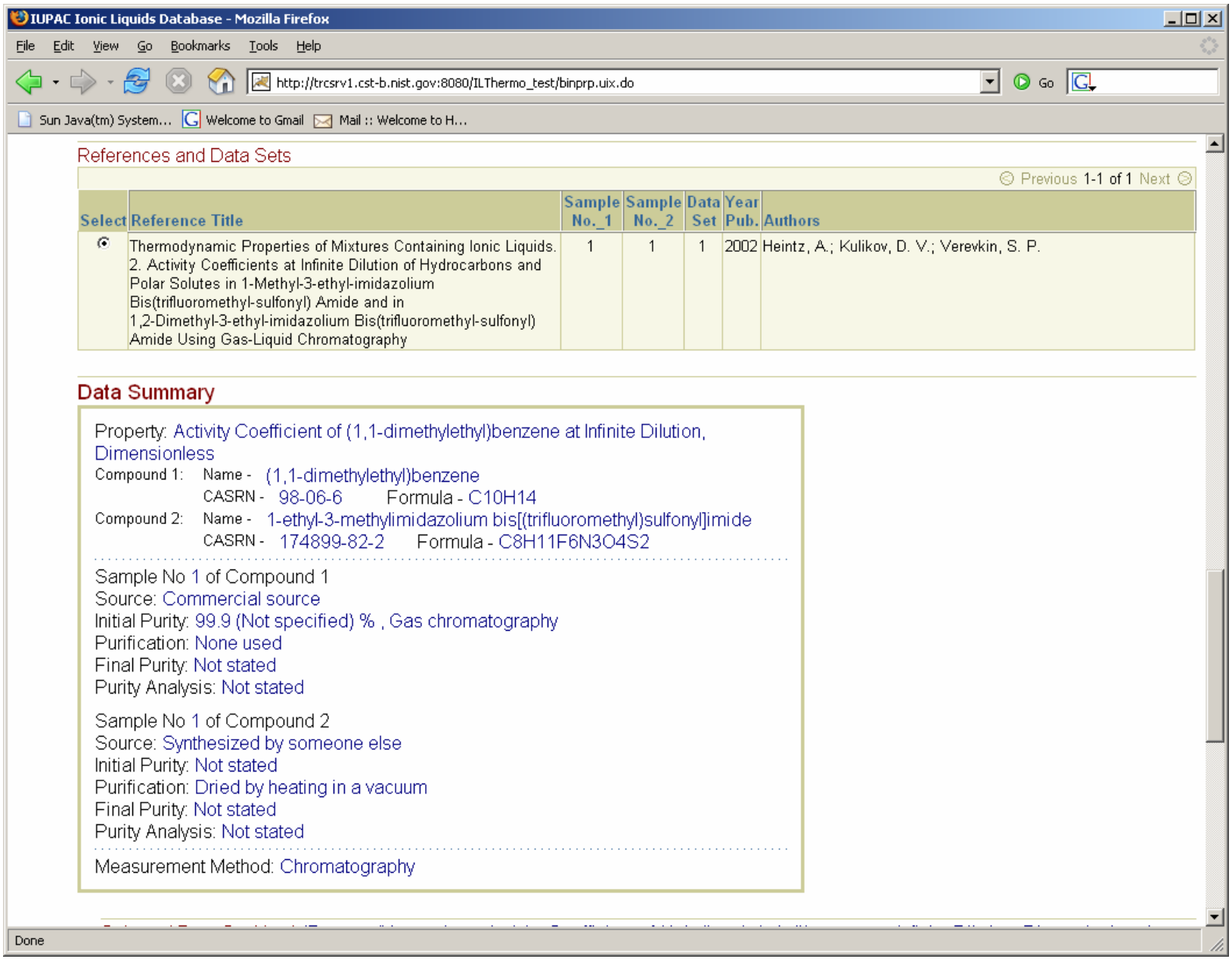


Binary Systems having: Activity Coefficient of Component 1 at Infinite Dilution, Dimensionless

Previous 1-20 of 510 Next 20

Select	Compound 1	Compound 2	References	Data Points
◉	(1,1-dimethylethyl)benzene	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	(1,1-dimethylethyl)benzene	1-butyl-4-methylpyridinium tetrafluorborate	1	4
○	(1,1-dimethylethyl)benzene	1-ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	(1-methylethenyl)benzene	1-butyl-4-methylpyridinium tetrafluorborate	1	4
○	(1-methylethenyl)benzene	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	(1-methylethenyl)benzene	1-ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	(RS)-2-butanol	1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	(RS)-2-butanol	1-butyl-4-methylpyridinium tetrafluorborate	1	4
○	(RS)-2-butanol	1-ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	(RS)-2-butanol	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	1,1-dimethylethyl methyl ether	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	1,1-dimethylethyl methyl ether	1-butyl-4-methylpyridinium tetrafluorborate	1	4
○	1,1-dimethylethyl methyl ether	1-ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	1,2-dichloroethane	1-ethyl-3-methylimidazolium tetrafluoroborate	1	2
○	1,2-dichloroethane	1-methyl-3-octylimidazolium tetrafluoroborate	1	2
○	1,2-dichloroethane	1-hexyl-3-methylimidazolium tetrafluoroborate	1	2
○	1,2-dichloroethane	1-butyl-3-methylimidazolium tetrafluoroborate	1	2
○	1,2-dimethylbenzene	1-octyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	1,2-dimethylbenzene	1-ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4
○	1,2-dimethylbenzene	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	1	4

Previous 1-20 of 510 Next 20


IUPAC Ionic Liquids Database - Mozilla Firefox
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http://trcsrv1.cst-b.nist.gov:8080/ILThermo_test/binprp.uix.do
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References and Data Sets
Previous 1-1 of 1 Next
Select
Reference Title
Sample No._1
Sample No._2
Data Set
Year Pub.
Authors
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 2. Activity Coefficients at Infinite Dilution of Hydrocarbons and Polar Solutes in 1-Methyl-3-ethyl-imidazolium Bis(trifluoromethyl-sulfonyl) Amide and in 1,2-Dimethyl-3-ethyl-imidazolium Bis(trifluoromethyl-sulfonyl) Amide Using Gas-Liquid Chromatography
1
1
1
2002
Heintz, A.; Kulikov, D. V.; Verevkin, S. P.
Data Summary
Property: Activity Coefficient of (1,1-dimethylethyl)benzene at Infinite Dilution, Dimensionless
Compound 1: Name - (1,1-dimethylethyl)benzene
CASRN - 98-06-6 Formula - C10H14
Compound 2: Name - 1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide
CASRN - 174899-82-2 Formula - C8H11F6N3O4S2
Sample No 1 of Compound 1
Source: Commercial source
Initial Purity: 99.9 (Not specified) % , Gas chromatography
Purification: None used
Final Purity: Not stated
Purity Analysis: Not stated
Sample No 1 of Compound 2
Source: Synthesized by someone else
Initial Purity: Not stated
Purification: Dried by heating in a vacuum
Final Purity: Not stated
Purity Analysis: Not stated
Measurement Method: Chromatography
Done

IUPAC Ionic Liquids Database - Mozilla Firefox

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http://trcsrv1.cst-b.nist.gov:8080/ILThermo_test/binprp.uix.do

Sun Java(tm) System... Welcome to Gmail Mail :: Welcome to H...

Measurement Method: Chromatography

Selected Data Set No. 1 (Property/Uncertainty - Activity Coefficient of (1,1-dimethylethyl)benzene at Infinite Dilution, Dimensionless)
Under System Condition(s): Pressure: 1 atm

Previous 1-4 of 4 Next

Temperature, K	Activity Coefficient of (1,1-dimethylethyl)benzene at Infinite Dilution, Dimensionless	Uncertainty Assigned by ILThermo
	Liquid	About Assigned Uncertainty
313	5.274	0.36
323	5.208	0.36
333	5.114	0.35
343	5.013	0.34

Selected Reference

Year Pub.	Authors	Source
2002	Heintz, A.; Kulikov, D. V.; Verevkin, S. P.	J. Chem. Eng. Data 47 , 894-899

Title:
Thermodynamic Properties of Mixtures Containing Ionic Liquids. 2. Activity Coefficients at Infinite Dilution of Hydrocarbons and Polar Solutes in 1-Methyl-3-ethyl-imidazolium Bis(trifluoromethyl-sulfonyl) Amide and in 1,2-Dimethyl-3-ethyl-imidazolium Bis(trifluoromethyl-sulfonyl) Amide Using Gas-Liquid Chromatography

Keywords:

Abstract:
Activity coefficients at infinite dilution ci yen of alkanes, alkenes, and alkylbenzenes as well as of the linear and branched C1-C6 alcohols, acetone, acetonitrile, ethyl acetate, alkyl ethers, and chloromethanes in the ionic liquids 1-methyl-3-ethyl-imidazolium bis(trifluoromethyl-sulfonyl) amide and 1,2-dimethyl-3- ethyl-imidazolium bis(trifluoromethyl-sulfonyl) amide were determined by gas chromatography using the ionic liquids as the stationary phase. The measurements were carried out at different temperatures between 313 K and 363 K. From the temperature dependence of the limiting activity coefficients partial molar excess enthalpies at infinite dilution Hi E,yen of the solutes in the ionic liquids have been derived.

Main Menu | Pure | **Binary** | Ternary | Contact us | Help

Done

Ionic Liquids Database- (ILThermo)

STATISTICAL INFORMATION ON ILTHERMO AS OF
10/05/2006

Total number of ions: 204

Total number of ionic liquids: 320

Total number of properties for pure ionic liquids: 21

Total number of properties for binary systems: 33

Total number of properties for ternary systems: 22

Total number of references: 155

Number of pure ionic liquids with property data: 111

Number of binary systems with property data: 875

Number of ternary systems with property data: 137

Total data points of property data for pure ionic liquids: 6674

Total data points of property data for binary systems: 16009

Total data points of property data for ternary systems: 2828

Total data points for all ionic liquids systems: 25511

Future Directions

- Populate *ILThermo* with the aim of creating a comprehensive database for IL properties
  - Collect and scan to PDF non-traditional sources of IL property data
  - Collect/ scan sources of molten salt property data
- Create links to other sources of information, when feasible, including:
  - Synthesis information
  - Manufacturer information
  - Others to be determined
- Examine feasibility of coordinating with other database developers.

Acknowledgements

- **NIST Management (Support)**
  - Dr. Daniel Friend
  - Dr. Gregory Rosasco (retired)
- **Other IUPAC Database Team Members**
  - Prof. Kenneth Seddon
  - Dr. Anthony Burgess
  - Prof. Marcelle Gaune-Escard
  - Prof. Andreas Heintz (and Dr. Sergey Verevkin)
  - Prof. Roger Sheldon
- **Presentation Graphics**
  - Ms. Marilyn Yetzbacher
  - Ms. Lorene Celano

Back Up Slides

Outline

- Need for open-access, public-domain, comprehensive data retrieval system
- IUPAC Task Group
- Supporting NIST infrastructure for a distributed access information system
- Database process flow
- ThermoML
- ILThermo – for thermodynamic, thermochemical, thermophysical and reaction data
- Web-based search & information retrieval
- Reports of Task Group activity
- Action items
- Future directions

Research Needs

NATO Advanced Research Workshop
Heraklion, Greece April, 2000

- **Toxicity, biodegradation, bio-accumulation, safety, health, and environment impact data.**
- **Cost/benefit, economic, and life-cycle analyses.**
- **A verified, web-based database of physical, thermodynamic, and related data (not process specific)**
- **Increase the number, but especially the areas of expertise of ionic liquids researchers.**

1st IUPAC Workshop on Ionic Liquids

17th IUPAC Conference on Chemical Themodynamics
Rostock, Germany July 28 to August 2, 2002

- Panel: K. Seddon, J. Brennecke, K. Marsh, J. Magee
- Typical Anions: X^-, where X=Cl,Br,I ; $[BF_4]^-$; $[PF_6]^-$; $[CF_3SO_3]^-$; $[N(OTP)_2]^-$; $[RCO_2]^-$; $[N(CN)_2]^-$; $[C_6H_5CO_2]^-$; $[RPO_2]^-$; [tartrate]$^-$; lactate]$^-$; $[RSO_3]^-$; $[NO_3]^-$; $[HSO_4]^-$; $[AlCl_4]^-$ (unstable)
- For fundamental understanding and industrial applications:$[N(OTP)_2]^-$; $[NO_3]^-$; Cl^-
- For fundamental understanding only: $[PF_6]^-$; $[BF_4]^-$; $[CF_3SO_3]^-$
- Typical Cations: $[Rmim]^+$; $[Rpy]^+$; $[NR_4]^+$; $[pyrolidinium]^+$
- A sample must be characterized for purity, esp. H_2O and Cl^- ion concentrations before and after measurements
- A Round-Robin measurement project was recommended
- Investigations of the effect of impurities on properties are needed
- Protocols for synthesis and purification are needed
- Standards for purity determination are needed

1st IUPAC Workshop (cont.)

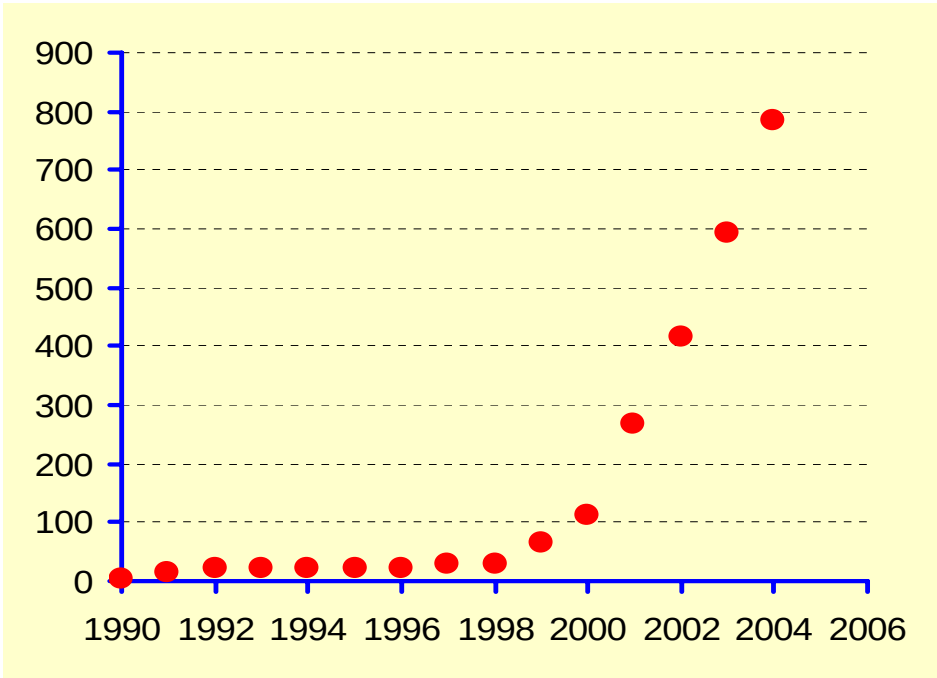
- Properties of pure components: Density (*T*); Viscosity (*T*); Isobaric heat capacity (*T*); Speed of sound (*T*); Thermal conductivity (*T*); Refractive index (*T*); Electrical conductivity; Surface tension; Vapor pressure (*T*); X-ray diffraction; Neutron diffraction; N.M.R. / I.R.; Melting point/phase diagram; Glass transition temperature; Enthalpies of fusion; Lattice energy; Dielectric constant
- Properties of mixtures, including ionic liquid + ionic liquid, ionic liquid + molecular compound (water, alcohols, aliphatic alkanes, aromatic hydrocarbons, halocarbons; gases) and ternary systems: Solubility; Activity coefficients at infinite dilution; Enthalpies of mixing; Gas solubilities; Partitioning coefficients (octanol/water)
- Kinetic studies are recommended
- A properties database is recommended; contributors should characterize the purity of their sample and the uncertainties in their data

1st IUPAC Workshop (cont.)

- IUPAC has approved support for a series of three workshops, with the second to be held at ICCT-2004 (Beijing) and ICCT-2006 (Boulder); *Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems* Project Task Group: K. Marsh (Chair), A. Heintz, J. Magee, M. Frenkel, K. Seddon, J. Brennecke and L. Rebelo
- IUPAC has approved support for the development of an ionic liquids database; *Ionic Liquids Database* Project Task Group: J. Magee, M. Frenkel, K. Marsh, K. Seddon (Chair), A. Heintz, M. Gaune-Escard, R. Sheldon and A. Burgess
- A database will be significantly more inclusive than NIST Standard Reference Database 27: NIST Molten Salts Database that provides molten state properties (density, surface tension, viscosity, electrical conductance) for 320 inorganic salts and 4,000 mixtures

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**

I U P A C

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Physical and Biophysical Chemistry Division (I)

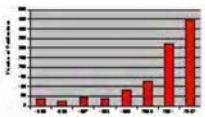
Number: 2003-020-2-100

Title: Ionic liquids database

Task Group
Chairman: K.R. Seddon

Members: Andrew Burgess, Michael Frenkel, Marcelle Gaune-Escard, Andreas Heintz, Joseph Magee, Kenneth Marsh, and Roger Sheldon

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.

Description:

Ionic liquids are expanding dramatically in popularity (see inset figure), and the first industrial application (the BASF BASIL process) was announced at the end of March 2003.
Crucial to their implementation on a wider scale (and these are green solvents) is universal access to their physical properties. As there are potentially over one million simple ionic liquids (although fewer than one thousand have yet been reported), the need for a living database, with continuous updating is paramount. This project brings together some of the world leaders in ionic liquid technology with leading thermodynamicists and database technologists.

A task group, that wishes to work under the auspices of IUPAC, has been formed to address the need for international scientific cooperation to implement the design and development of a web-based free-access database for

1st Task Group Meeting

Delft University of Technology
Delft, Netherlands January 26, 2004

- Present: Andrew Burgess, Marcelle Gaune-Escard, Michael Frenkel, Joseph Magee, Kenneth Marsh, Kenneth Seddon, Roger Sheldon (host), Sergey Verevkin (for Andreas Heintz)
- A distributed access database would be developed with various types of data being independently managed
- Coverage would include synthesis, catalysis, structure, manufacturing, modeling as well as physical and chemical property data
- New required fields in the primary database were defined including those for handling polymers and enzymes
- Ensuring complementarity with high-temperature molten salt data and the QUILL database, avoiding duplication of effort

Minutes of First Ionic Liquids Database Meeting
(#2003-020-2-100)
Delft University of Technology, 26th January 2004

Present: Andrew Burgess, Marcelle Gaune-Escard, Michael Frenkel, Joseph W. Magee, Kenneth N. Marsh, Kenneth Richard Seddon, Roger Sheldon, Sergey P. Verevkin (standing in for Andreas Heintz)

Opening Remarks

The Committee expressed their thanks to Prof. Sheldon for hosting the meeting.

NIST Database Projects

Drs. Magee and Frenkel gave a detailed presentation on the structure and input methods for extant NIST databases. In particular, the relationship between the primary NIST thermodynamic database and the new ionic liquid database was explored; the product should be exportable to Aspen. The importance of the ionic liquid workshop at the 17th IUPAC Conference on Chemical Thermodynamics in Rostock, Germany, 28th July to 2nd August, 2002 in defining the current project was noted. The slides are attached as an Appendix to this report.

Discussion

1. New Required Fields

The requirements of ionic materials, as compared with molecular systems, mean that new fields in the primary database need to be defined. The absolute minimum basic requirements are:

- Stoicheiometry of salt
- Name of anion
- CAS registry number of anion
- Name of cation
- CAS registry number of cation
- Electrical conductivity

Desirable extra fields would be:

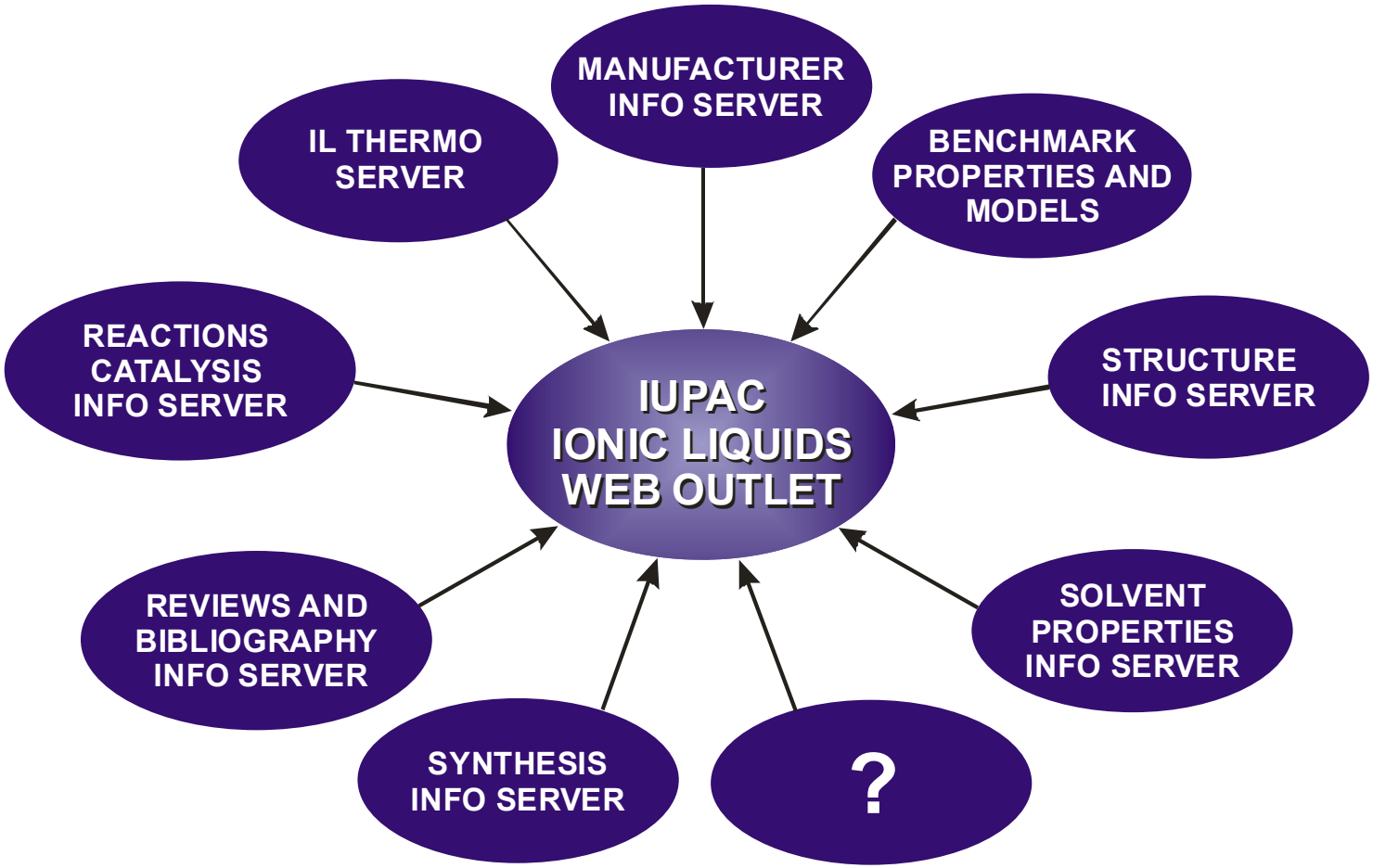
- Lattice energy (both theoretical and "experimental")
- Dielectric constant (frequency dependent)
- Oxygen sensitivity (Boolean)
- Water sensitivity (Boolean)
- Corrosion data (text file)
- Solubility data (Boolean)
- Enzyme activation (Boolean)
- Items to be inserted into the QUILL structural and spectroscopic database:
- X-ray structural data
- Neutron structural data
- EXAFS structural data
- Spectroscopic data (MS, NMR, IR, Raman, *etc.*)
- Thermal data (TGA, DSC)
- Toxicity data

Images are most conveniently incorporated as jpeg files.

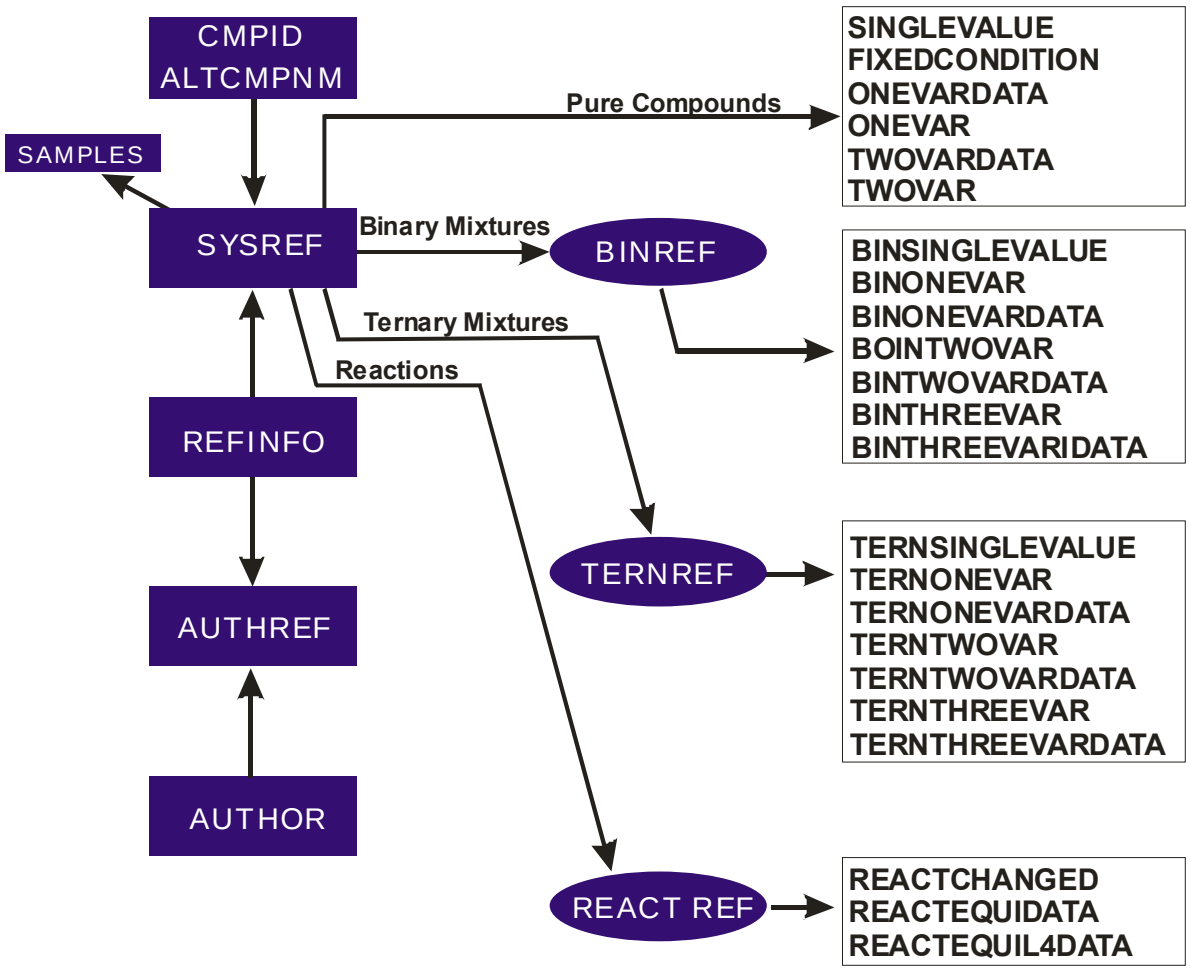
Vision for the Ionic Liquids Database

- Searchable Web-based database residing on a NIST-Thermodynamics Research Center server
- Experimental and predicted data for thermodynamic, thermochemical and transport properties with their associated uncertainties
- Recommended benchmark data for selected ionic liquids and mixtures
- Recommended protocols for synthesis, purification, purity determination and sample handling procedures
- Structure, theoretical studies, solvent properties and reactions, catalytic properties, reviews, and a bibliography
- Models fitted to the most reliable property data
- Quantitative structure-property models for prediction of properties
- The auspices of IUPAC will promote a broad-based international effort to collect all relevant information

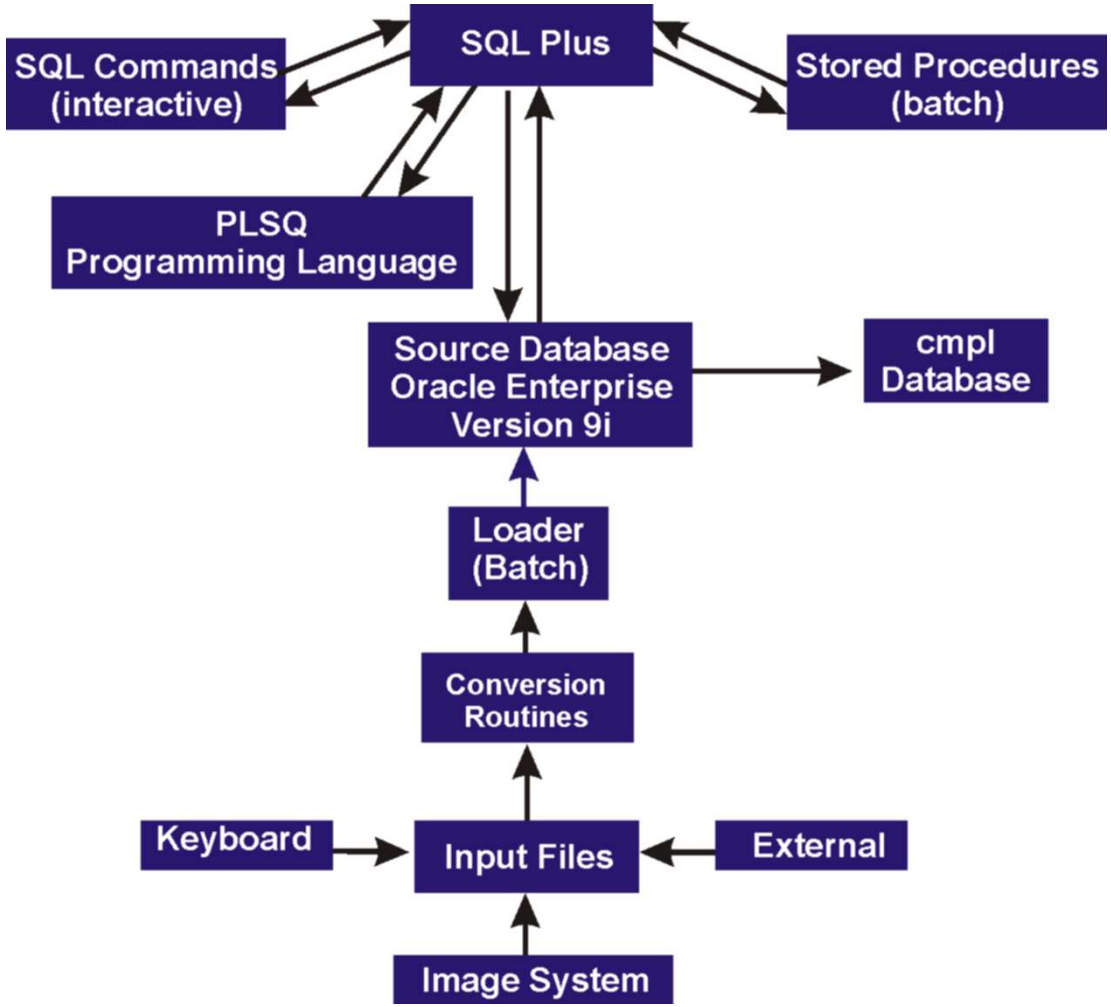
Distributed Ionic Liquids Information Access



Source Database Tables

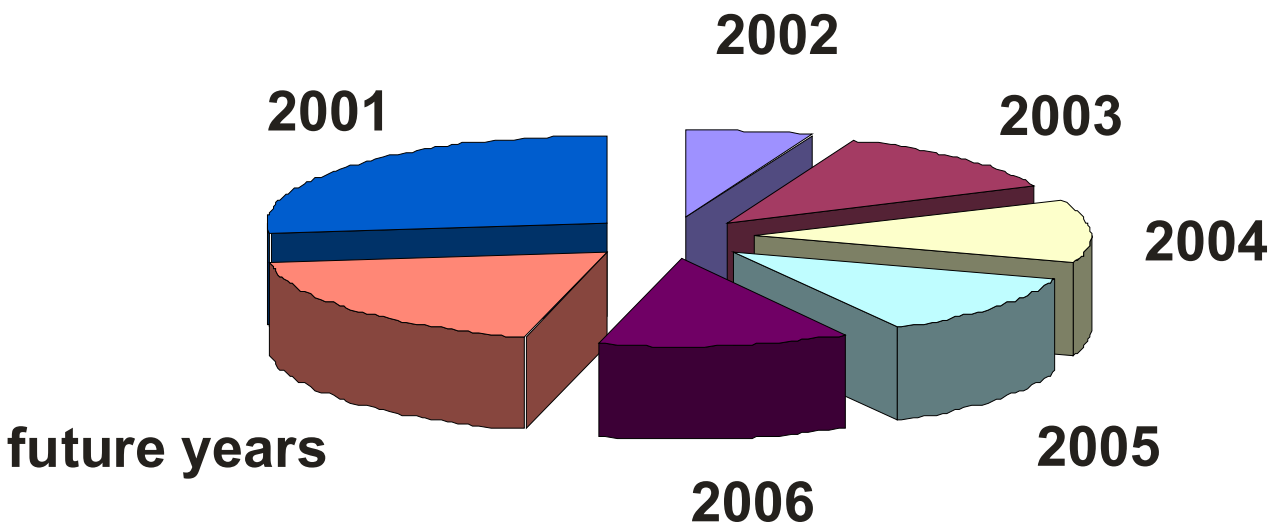


Database Utilities on the Server

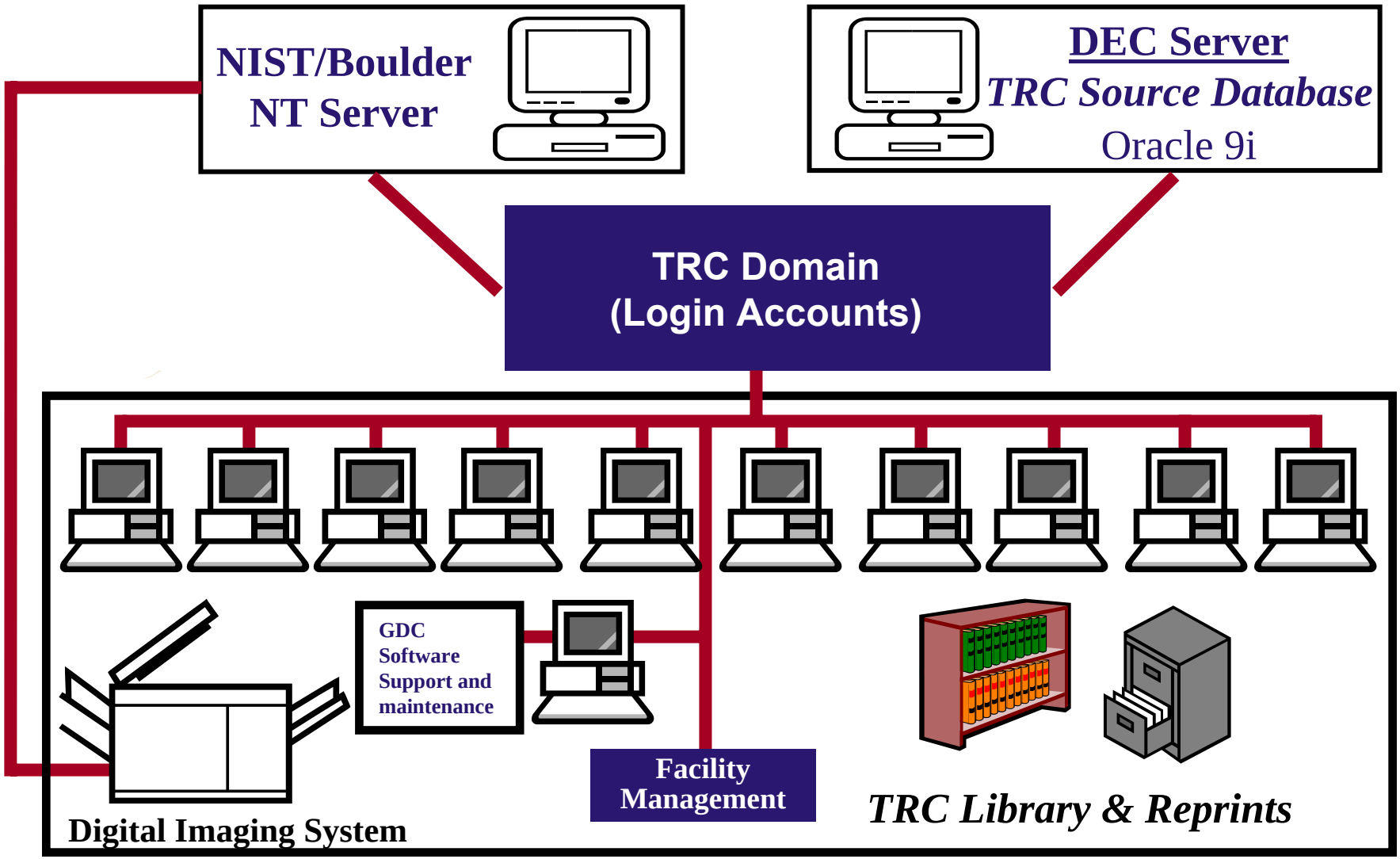


SOURCE DATA ENTRY
PLANNED PROGRESS

TARGET: 3 MILLION DATA POINTS BY 2006



TRC Data Entry Facility: Equipment



Description of GDC Software

J. Chem. Inf. Comput. Sci. **2003,** *43,* 15−24

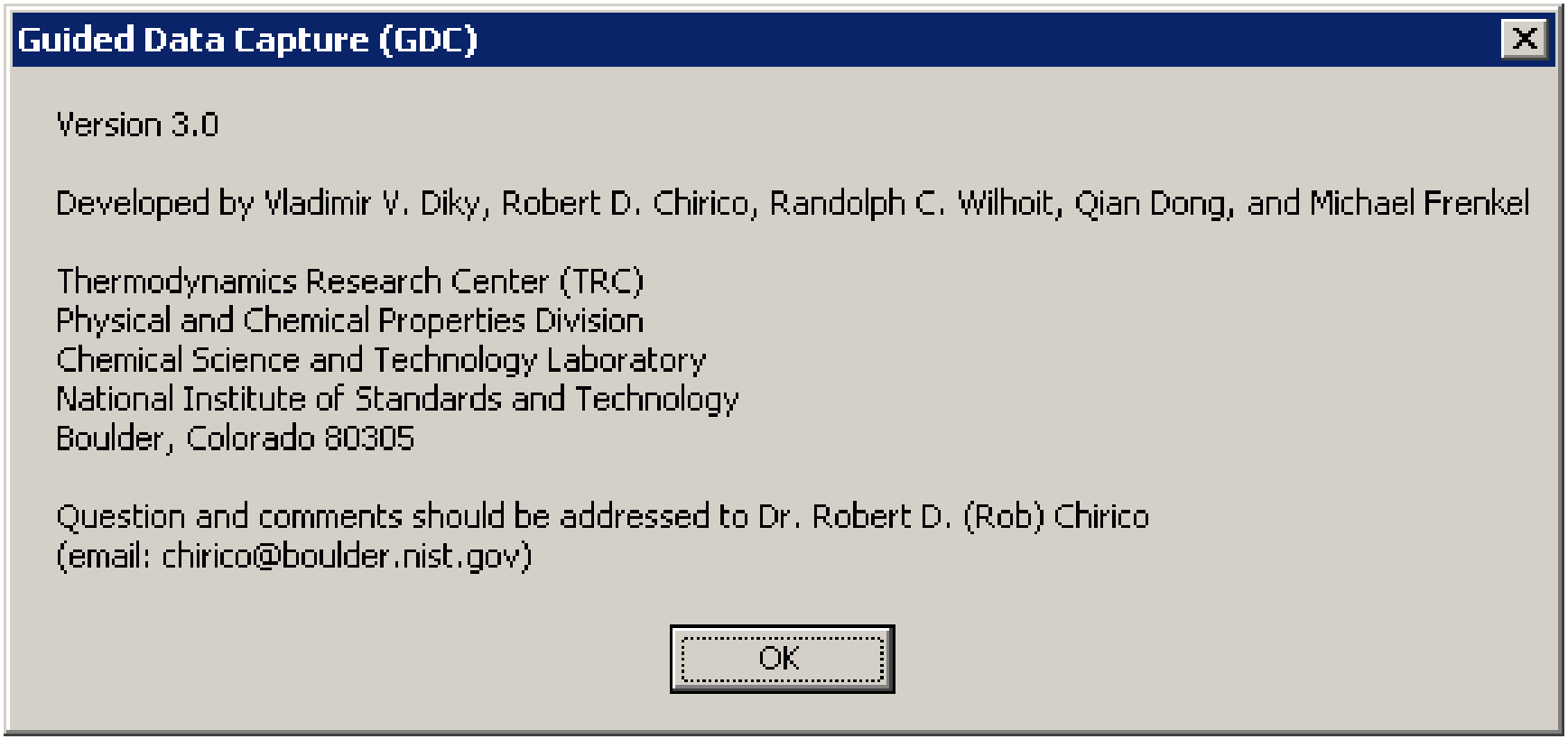
Windows-Based Guided Data Capture Software for Mass-Scale Thermophysical and Thermochemical Property Data Collection†

Vladimir V. Diky, Robert D. Chirico,* Randolph C. Wilhoit, Qian Dong, and Michael Frenkel

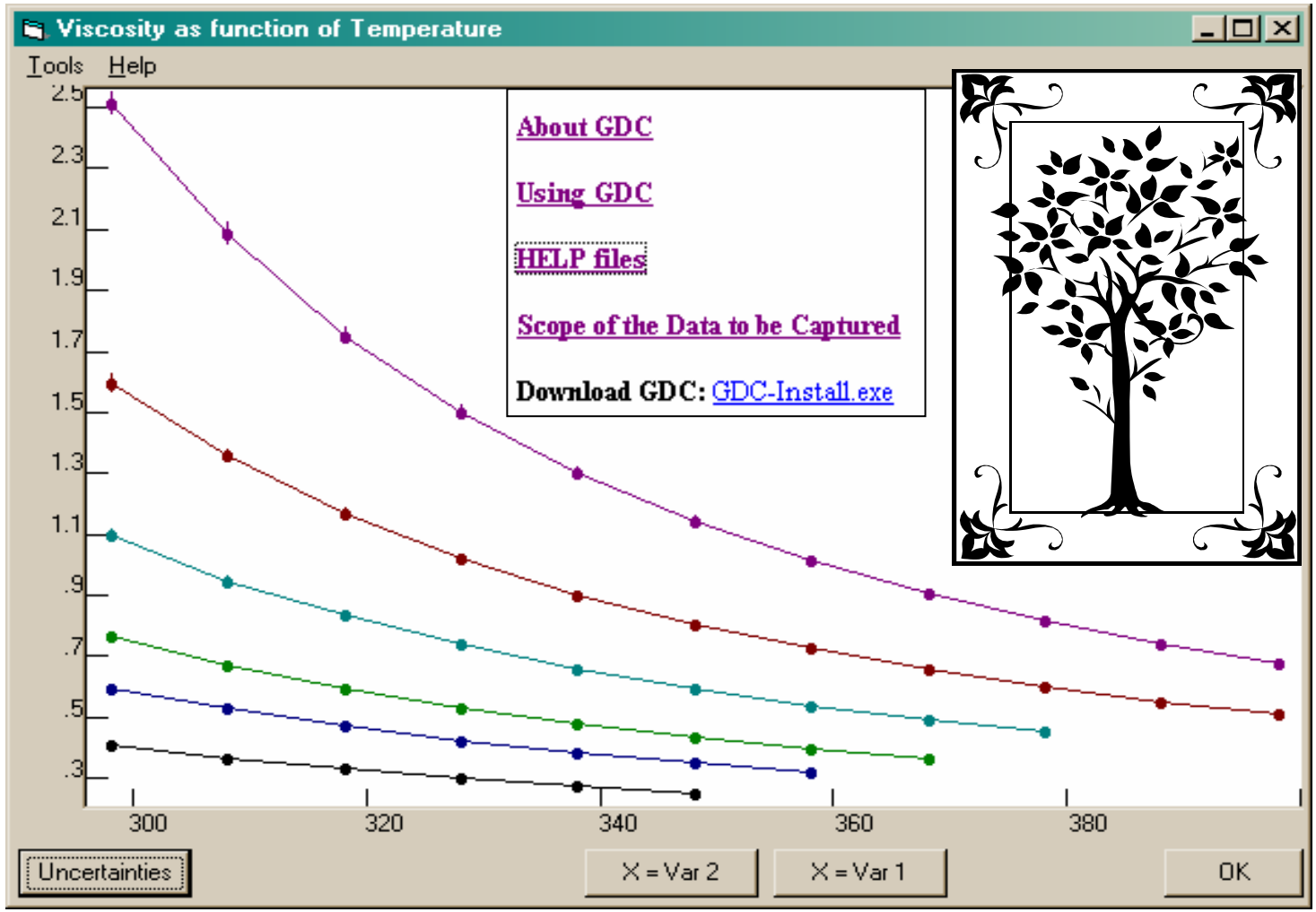
Thermodynamics Research Center, National Institute of Standards and Technology (NIST), Boulder, Colorado 80305-3328

Received May 7, 2002

Guided data capture software (GDC) is described for mass-scale abstraction from the literature of experimental thermophysical and thermochemical property data for organic chemical systems involving one, two, and three components, chemical reactions, and chemical equilibria. Property values are captured with a strictly hierarchical system based upon rigorous application of the thermodynamic constraints of the Gibbs phase rule with full traceability to source documents. Key features of the program and its adherence to scientific principles are described with particular emphasis on data-quality issues, both in terms of data accuracy and database integrity.

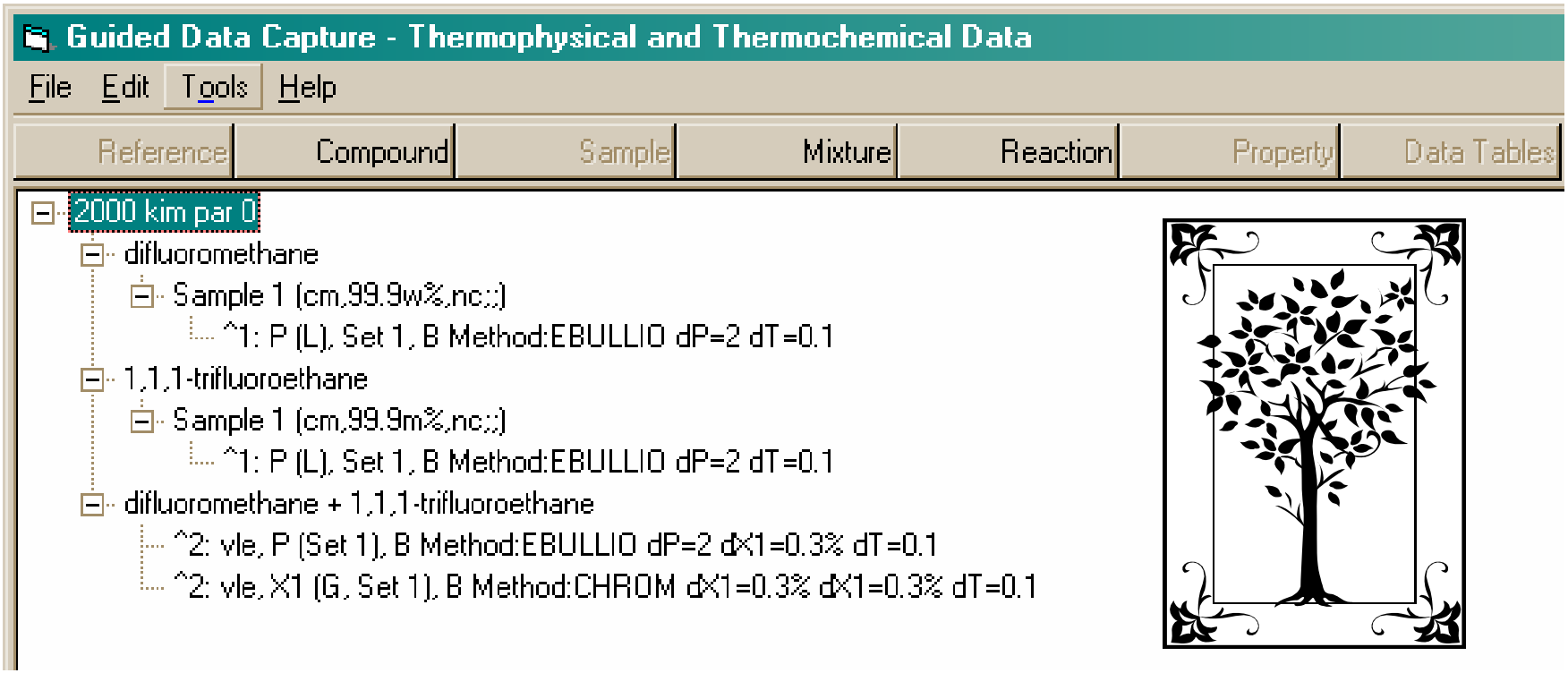

Guided Data Capture (GDC)
Version 3.0
Developed by Vladimir V. Diky, Robert D. Chirico, Randolph C. Wilhoit, Qian Dong, and Michael Frenkel
Thermodynamics Research Center (TRC)
Physical and Chemical Properties Division
Chemical Science and Technology Laboratory
National Institute of Standards and Technology
Boulder, Colorado 80305
Question and comments should be addressed to Dr. Robert D. (Rob) Chirico
(email: chirico@boulder.nist.gov)
OK

GUIDED DATA CAPTURE Software

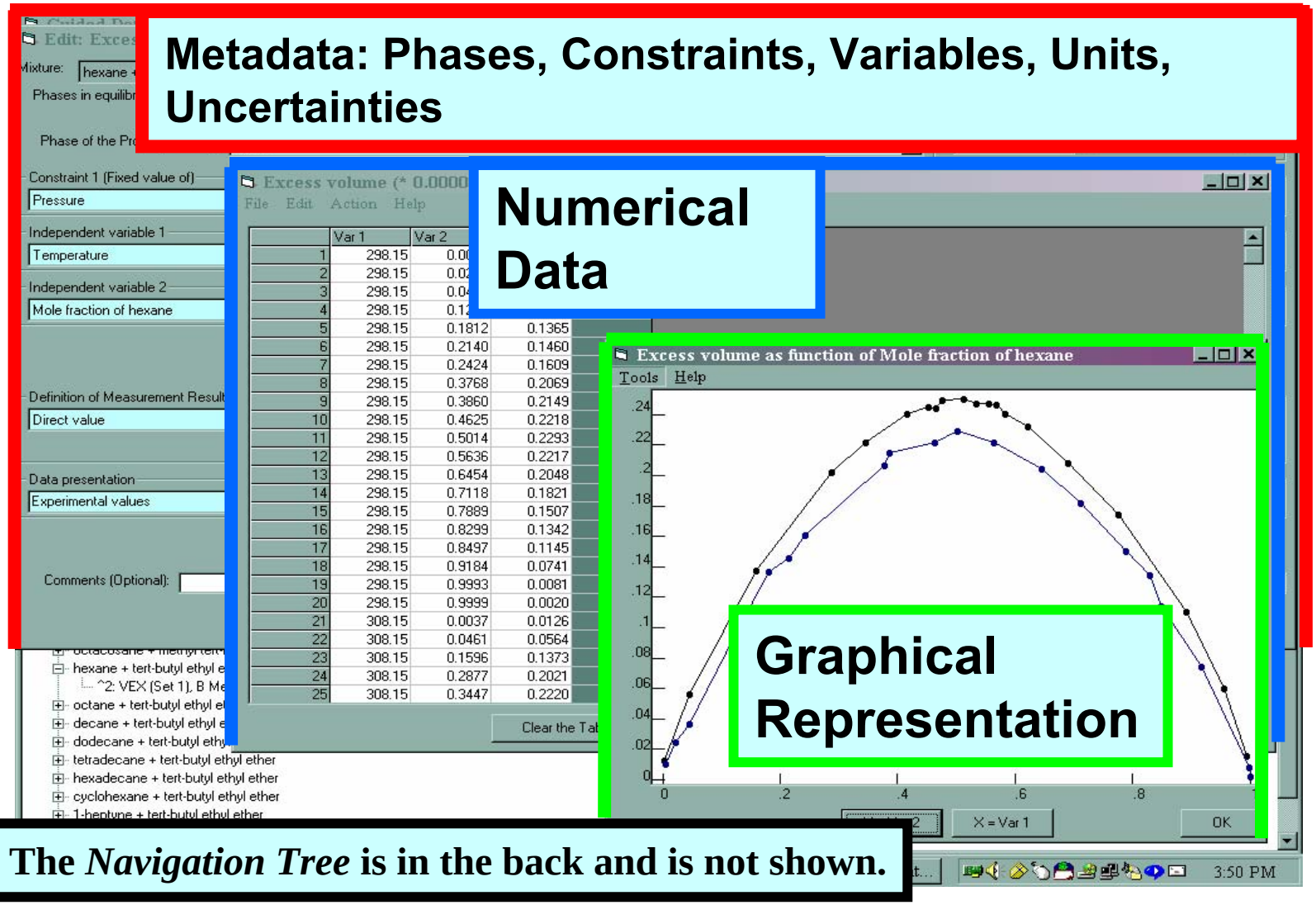


Navigation Tree: *("User Interface")*

- **Grows as info is added**
- **Any line can be accessed for editing**
- **Compound synonyms are available**



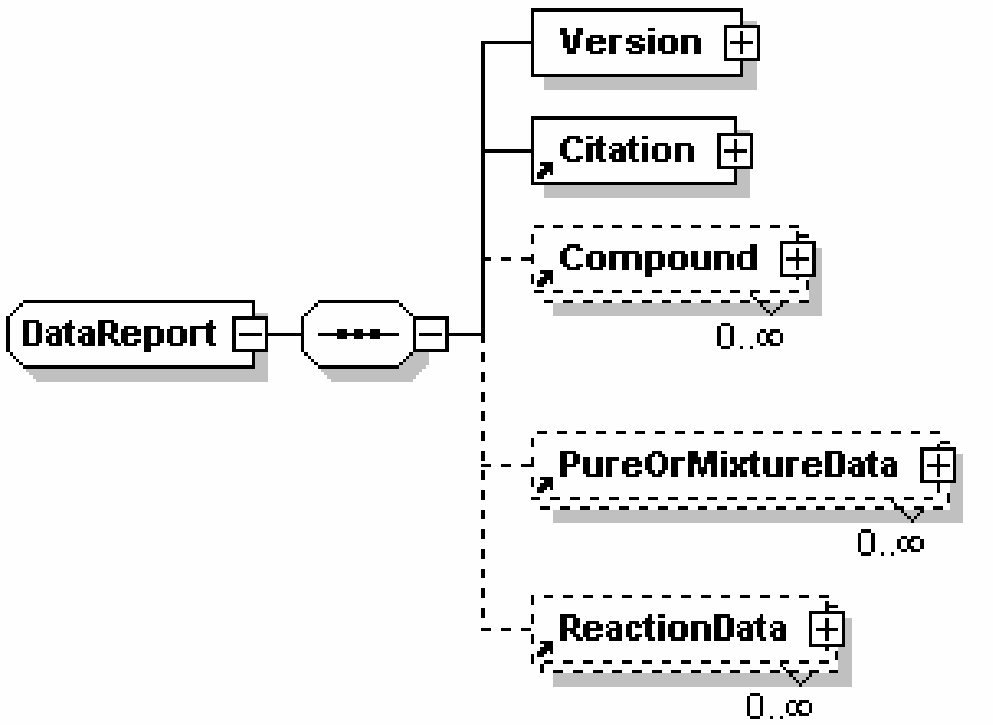

CSTL



	Var 1	Var 2	
1	298.15	0.00	
2	298.15	0.02	
3	298.15	0.04	
4	298.15	0.12	
5	298.15	0.1812	0.1365
6	298.15	0.2140	0.1460
7	298.15	0.2424	0.1609
8	298.15	0.3768	0.2069
9	298.15	0.3860	0.2149
10	298.15	0.4625	0.2218
11	298.15	0.5014	0.2293
12	298.15	0.5636	0.2217
13	298.15	0.6454	0.2048
14	298.15	0.7118	0.1821
15	298.15	0.7889	0.1507
16	298.15	0.8299	0.1342
17	298.15	0.8497	0.1145
18	298.15	0.9184	0.0741
19	298.15	0.9993	0.0081
20	298.15	0.9999	0.0020
21	308.15	0.0037	0.0126
22	308.15	0.0461	0.0564
23	308.15	0.1596	0.1373
24	308.15	0.2877	0.2021
25	308.15	0.3447	0.2220

The *Navigation Tree* is in the back and is not shown.

ThermoML: General Structure



ThermoML was developed in cooperation with DIPPR

Reviews

ThermoML—An XML-Based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 1. Experimental Data

Michael Frenkel,* Robert D. Chirico, Vladimir V. Diky, and Qian Dong

Thermodynamics Research Center (TRC), Physical and Chemical Properties Division, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305-3328

Svetlana Frenkel and Paul R. Franchois

Information Technology Laboratory, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305-3337

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Thomas L. Teague

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Kenneth N. Marsh

Department of Chemical and Process Engineering, University of Canterbury, Private Bag 4800, Christchurch, New Zealand

Randolph C. Wilhoit

Texas Experimental Engineering Station, Texas A&M University System, College Station, Texas 77843

Paper 2. Representation of *Uncertainties*

1344 *J. Chem. Eng. Data* **2003,** *48,* 1344−1359

ThermoML—An XML-Based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 2. Uncertainties

Robert D. Chirico,* Michael Frenkel, and Vladimir V. Diky

Thermodynamics Research Center (TRC), Physical and Chemical Properties Division, National Institute of Standards and Technology, 325 Broadway, Boulder, Colorado 80305-3328

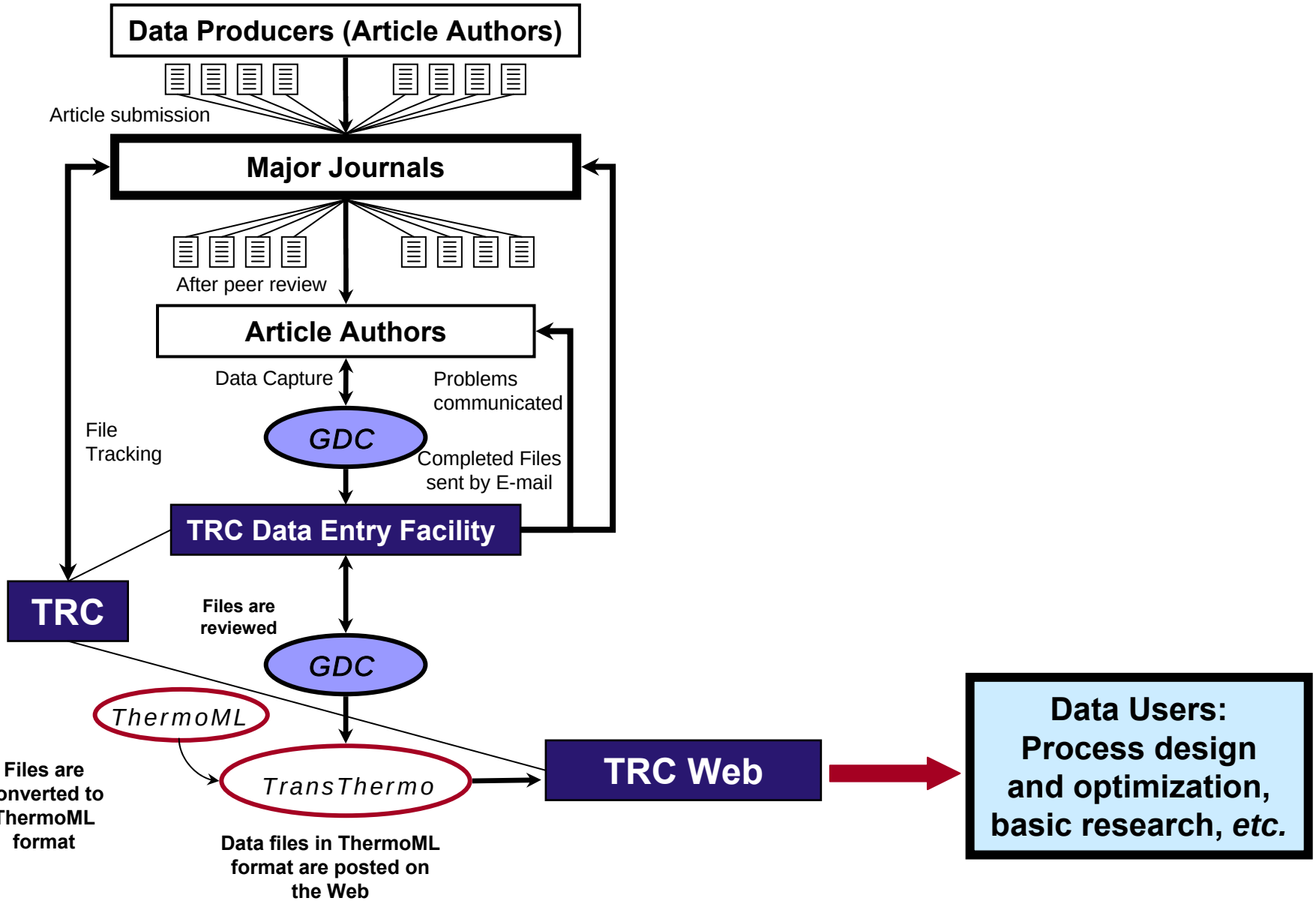
Kenneth N. Marsh

Department of Chemical and Process Engineering, University of Canterbury, Private Bag 4800, Christchurch, New Zealand

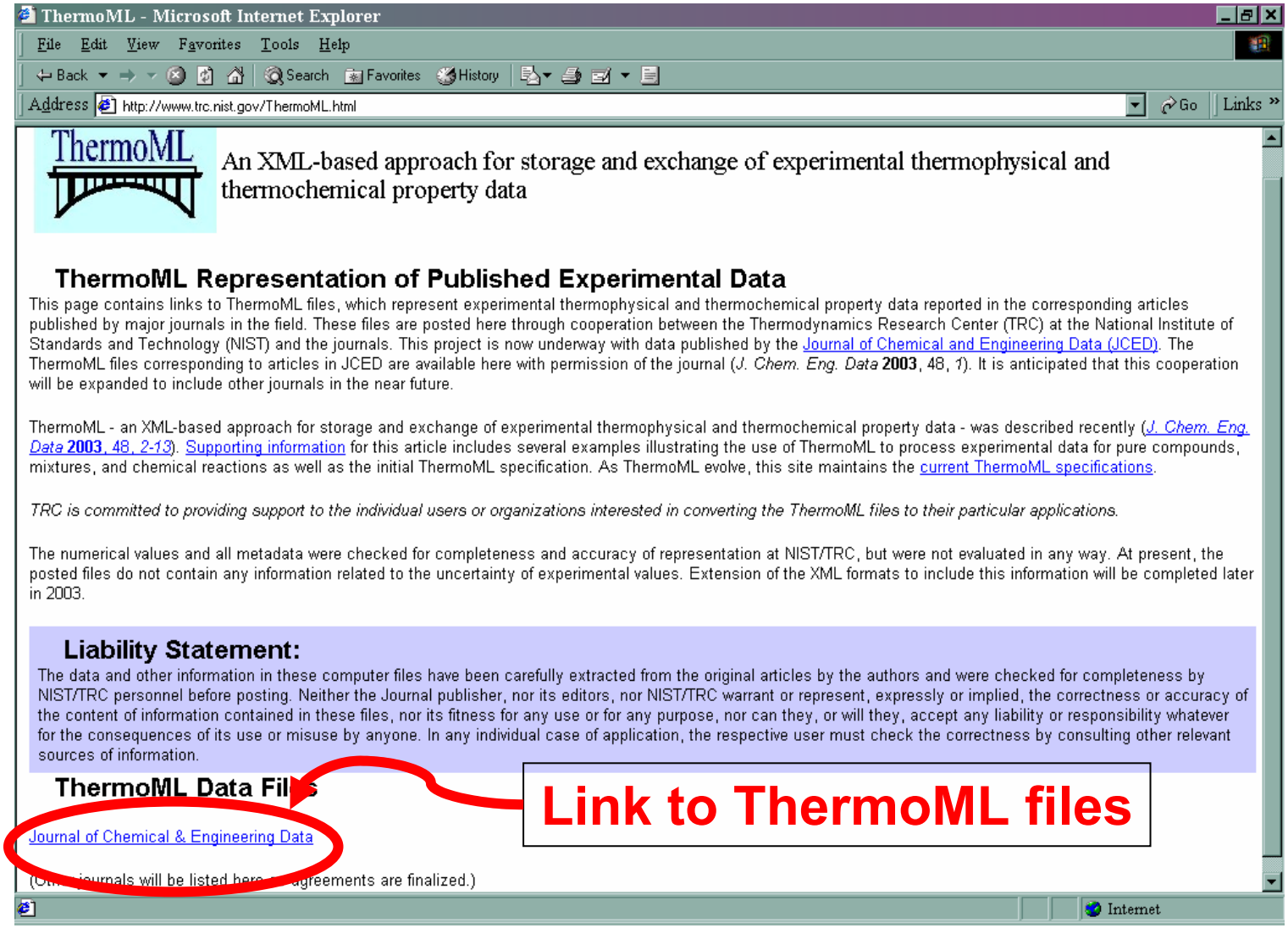
Randolph C. Wilhoit

Texas Experimental Engineering Station, Texas A&M University System, College Station, Texas 77843

ThermoML is an XML-based approach for storage and exchange of experimental and critically evaluated thermophysical and thermochemical property data. Extensions to the ThermoML schema for the expression of uncertainties are described. Basic principles, scope, and description of all new structural elements are discussed. Representation of upper and lower limits for property values is also addressed. ThermoML covers essentially all experimentally determined thermodynamic and transport property data (more than 120 properties) for pure compounds, multicomponent mixtures, and chemical reactions (including change-of-state and equilibrium). Properties of polymers and radicals and some properties of ionic systems are not represented at present. The present role of ThermoML in global data submission and dissemination is discussed with particular emphasis on cooperation between major journals in the field and the Thermodynamics Research Center (TRC) at the National Institute of Standards and Technology. The text of several data files illustrating the expression of uncertainties in ThermoML format for pure compounds, mixtures, and chemical reactions are provided as Supporting Information, as well as the complete updated ThermoML schema text.


Data Producers (Article Authors)
Article submission
Major Journals
After peer review
Article Authors
Data Capture
Problems communicated
File Tracking
GDC
Completed Files sent by E-mail
TRC Data Entry Facility
TRC
Files are reviewed
GDC
ThermoML
Files are converted to ThermoML format
TransThermo
Data files in ThermoML format are posted on the Web
TRC Web
Data Users: Process design and optimization, basic research, etc.

ThermoML Files are Posted on the Web



ThermoML Data for JCED - 2003 Vol. 48 Issue 2 - Microsoft Internet Explorer

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Address http://www.trc.nist.gov/data/jced/2003v48/i02/jced2003v48i02.html Go Links

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Journal of
Chemical & Engineering Data

Select Decade: Current | Select Volume: 2003/Vol. 48 | Select Issue Number: Iss. 2, pages 211-444 | Go

Iss .1, pages 1-210
Iss. 2, pages 211-444

ThermoML Data for the *Journal of Chemical & Engineering Data*, Vol. 48, No. 2 March 2003
Developed in cooperation between the *Journal of Chemical & Engineering Data* and the *Thermodynamics Research Center* (TRC)

Liquid-Liquid Equili… the Binary Systems of *N*-Formylmorpholine with Cycloalkanes
MinSu Ko, Sangyo… Na, Sungjin …e, and Hwayong Kim
pp 248 - 252; **(Article)**

ThermoML Data(To d…wnload: right-c…k on link and select "Save Link Target As")

…and Estimation of …enry's Law Constants of Chlorinated Ethylenes in Aqueous Surfactant Solutions
Tsutomu Shimotori and William A. Arn…
pp 253 - 261; **(Article)**

ThermoML Data(To download: right-click on li… and s…

Vapor Liquid Equilibria for Ethanol + 2,4,4-Trim… …entene at 101 kPa
Petri Uusi-Kyyny, Virpi Tarkiainen, Younghun Kim, Rain…
pp 280 - 285; **(Article)**

ThermoML Data(To download: right-click on link and select "Save Link Target As")

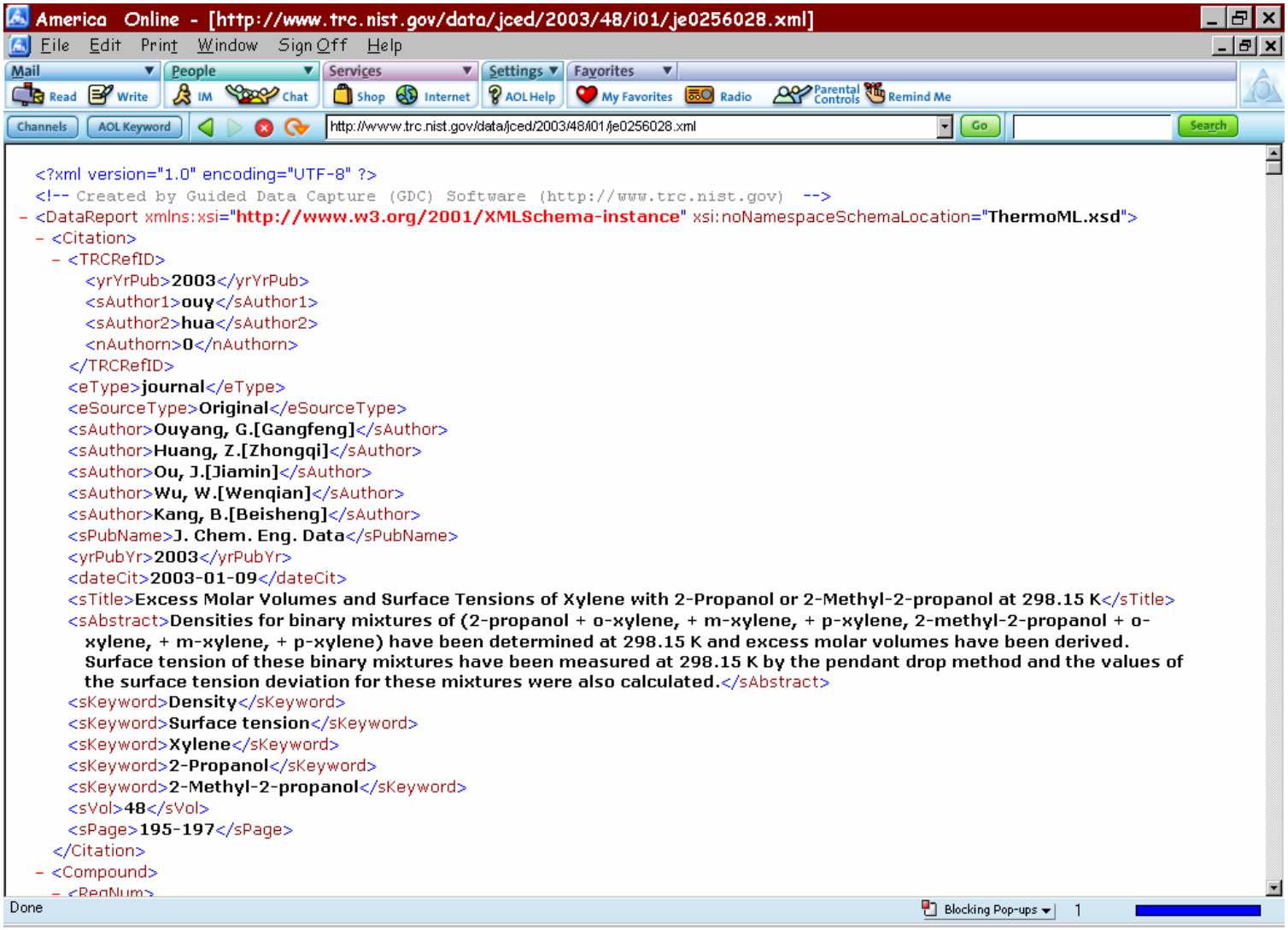
Vapor Liquid Equilibrium between (278.15 and 323.15) K and Excess Functions at *T* = 298.15 K for 1-Bromobutane with 2-Methyl-1-propanol or 2-Butanol
Santiago Martínez, Rosa Garriga, Pascual Pérez, and Mariano Gracia
pp 294 - 301; **(Article)**

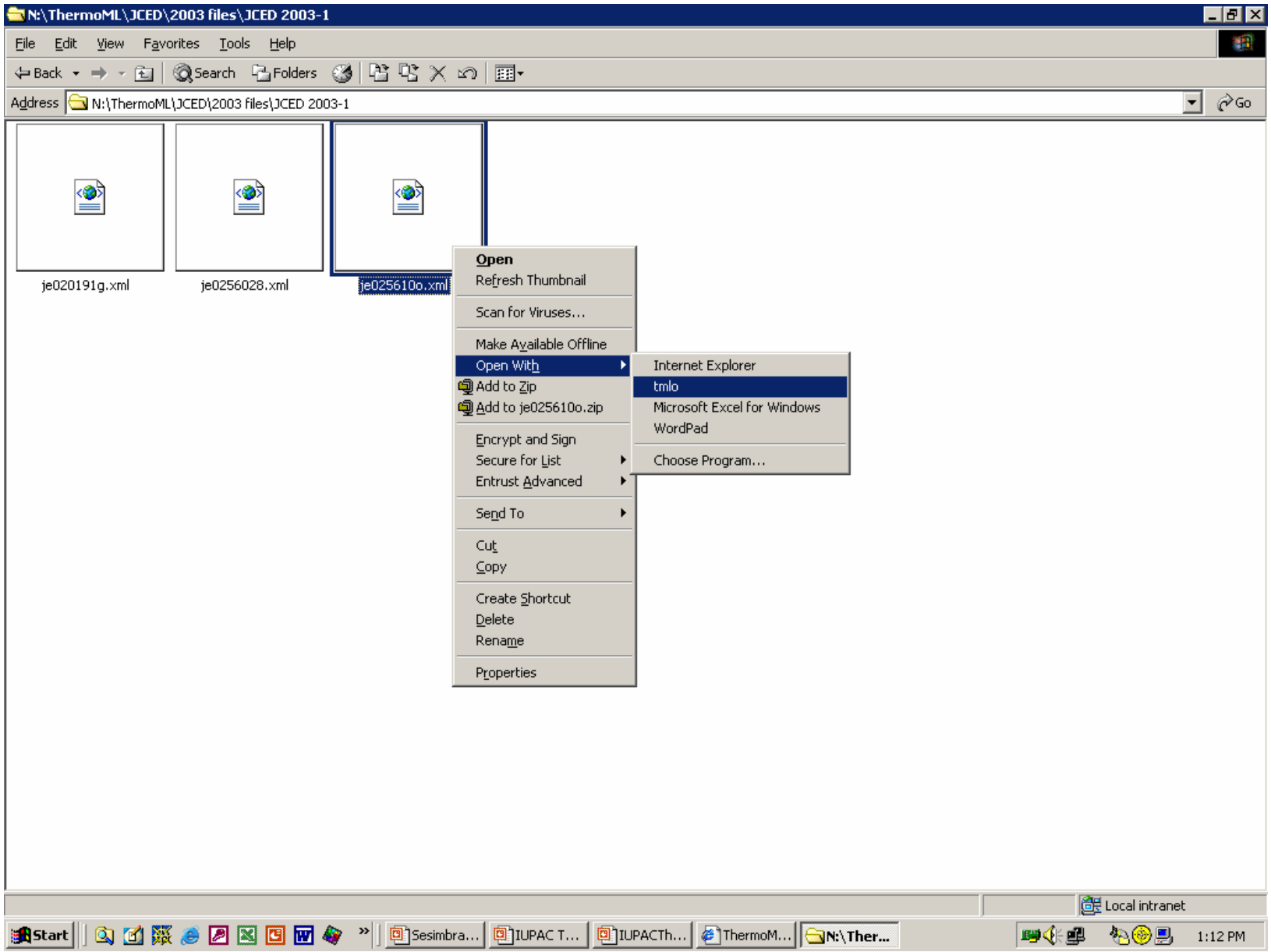
Done Internet

Link to *ThermoML* file for the individual article

2003 JCED:
Issue 1: 3 articles
Issue 2: 21 articles
Issue 3: 30 articles

A *ThermoML* file available for free download




N:\ThermoML\JCED\2003 files\JCED 2003-1
File Edit View Favorites Tools Help
Back Search Folders
Address N:\ThermoML\JCED\2003 files\JCED 2003-1
Go
je020191g.xml
je0256028.xml
je025610o.xml
Open
Refresh Thumbnail
Scan for Viruses...
Make Available Offline
Open With
Add to Zip
Add to je025610o.zip
Encrypt and Sign
Secure for List
Entrust Advanced
Send To
Cut
Copy
Create Shortcut
Delete
Rename
Properties
Internet Explorer
tmlo
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WordPad
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IUPAC T...
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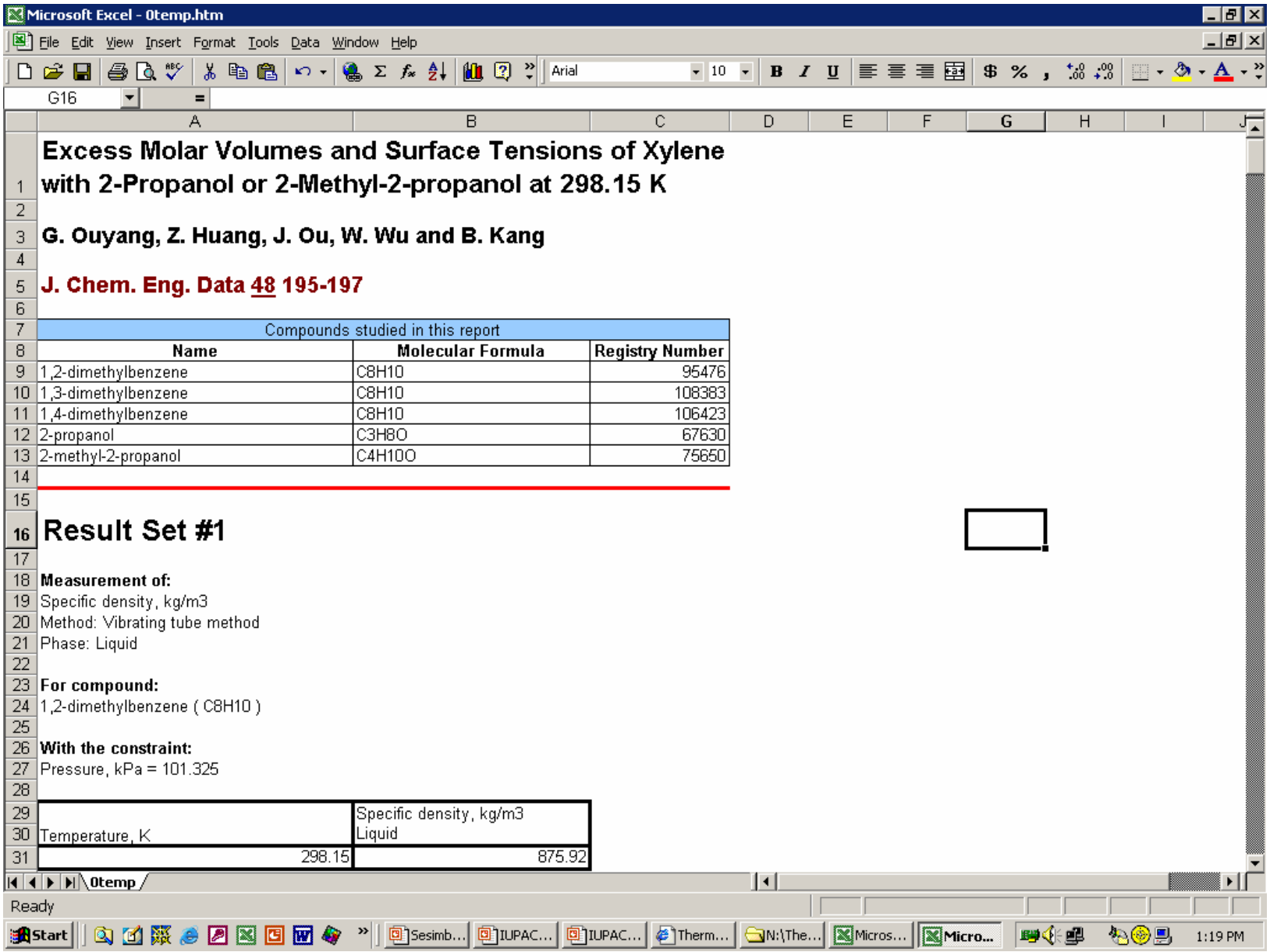

Microsoft Excel - 0temp.htm
File Edit View Insert Format Tools Data Window Help
Arial 10
G16
Excess Molar Volumes and Surface Tensions of Xylene with 2-Propanol or 2-Methyl-2-propanol at 298.15 K
G. Ouyang, Z. Huang, J. Ou, W. Wu and B. Kang
J. Chem. Eng. Data 48 195-197
Compounds studied in this report
Name | Molecular Formula | Registry Number
1,2-dimethylbenzene | C8H10 | 95476
1,3-dimethylbenzene | C8H10 | 108383
1,4-dimethylbenzene | C8H10 | 106423
2-propanol | C3H8O | 67630
2-methyl-2-propanol | C4H10O | 75650
Result Set #1
Measurement of:
Specific density, kg/m3
Method: Vibrating tube method
Phase: Liquid
For compound:
1,2-dimethylbenzene (C8H10)
With the constraint:
Pressure, kPa = 101.325
Temperature, K | Specific density, kg/m3 Liquid
298.15 | 875.92
0temp
Ready
Start
1:19 PM

International Union of Pure and Applied Chemistry - Netscape

File Edit View Go Window Help

Current Project

Committee on Printed and Electronic Publications

Number: 2002-055-3-024

Title: XML-based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture

Task Group
Chairman: M. Frenkel

Members: K.N. Marsh, W.A. Wakeham, J.H. Dymond, S. E. Stein, and E. Koenigsberger

Completion Date: 2004

Objective:
It is intended to create an XML-based dictionary for storage and exchange of thermophysical and thermochemical data based on

ThermoML - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites Media

Address http://www.iupac.org/namespaces/ThermoML/index.html Go Links

ThermoML - An XML-based IUPAC Standard for Thermodynamic Property Data

"ThermoML" is reserved namespace for the XML-based IUPAC standard for experimental and critically-evaluated thermodynamic property data storage and capture being developed under the IUPAC project 2002-055-3-024 (M. Frenkel, Task Group Chairman, J. H. Dymond, E. Koenigsberger, K. N. Marsh, S. E. Stein, W. A. Wakeham- members).

This project is conducted as one of the activities of the IUPAC Committee on Printed and Electronic Publications (CPEP), L. Glasser, Chairman; A. N. Davies, Secretary.

ThermoML covers essentially all experimentally determined thermodynamic and transport property data (more than 120 properties) for pure compounds, multicomponent mixtures, and chemical reactions (including change-of-state and equilibrium). Although the focus of ThermoML is properties determined by direct experimental measurement, ThermoML does cover key derived property data such as azeotropic properties, Henry's Law constants, virial coefficients (for pure compounds and mixtures), activities and activity coefficients, fugacities and fugacity coefficients, and standard properties derived from high-precision adiabatic heat-capacity calorimetry.

The ThermoML structure represents a balanced combination of hierarchical and relational elements. The ThermoML schema structure explicitly incorporates structural elements related to basic principles of phenomenological thermodynamics: thermochemical and thermophysical (equilibrium and transport) properties, state variables, system constraints, phases, and units. Meta- and numerical-data records are grouped into 'nested blocks' of information corresponding to data sets. The metadata records precede numerical data information, providing a robust foundation for generating 'header' records for any relational database where ThermoML-formatted files could be incorporated. The structural features of the ThermoML metadata records ensure unambiguous interpretation of numerical data as well as data-quality control based on the Gibbs Phase Rule.

The framework of the ThermoML has been described in details in the article "ThermoML - an XML-based Approach for Storage and Exchange of Experimental and Critically Evaluated Thermophysical and Thermochemical Property Data. 1. Experimental Data" by M. Frenkel, R. D. Chirico, V. V. Diky, Q. Dong, S. Frenkel, P. R. Franchois, D. L. Embry, T. L. Teague, K. N. Marsh, and R. C. Wilhoit, published in the *Journal of Chemical and Engineering Data* (**2003**, *48*, 2-13). The expression of uncertainty requires clear definition of a variety of quantities and terms. Expansion of the ThermoML framework for the expression of uncertainties of thermodynamic properties (including definitions and descriptions of the standard uncertainties, combined uncertainties, expanded uncertainties, and various measures of the precision) conform to the Guide to the Expression of Uncertainty in Measurement, ISO (International Organization for Standardization), October, 1993 as well as the U. S. Guide to the Expression of Uncertainty in Measurement. This expansion has been described in details in the article "ThermoML - an XML-based Approach for Storage and Exchange of Experimental

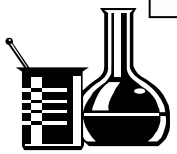
http://pubs.acs.org/cgi-bin/abstract.cgi/jceaax/2003/48/i01/abs/je025645o.html Internet

Global Data Communication Process

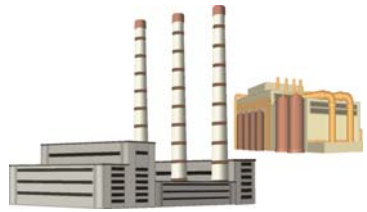
Committee on Printed & Electronic Publication (CPEP)

International Association of Chemical Thermodynamics (IACT)

IUPAC



Thermodynamicists



Industrial Engineers

Guided Data Capture (GDC)

"Reader" Software

Measurements

- J. Chem. Eng. Data *(ACS)*
- J. Chem. Thermodyn. *(Elsevier)*
- Fluid Phase Equilibria *(Elsevier)*
- Int. J. Thermophys. *(Kluwer)*
- Thermochimica Acta *(Elsevier)*

ThermoML

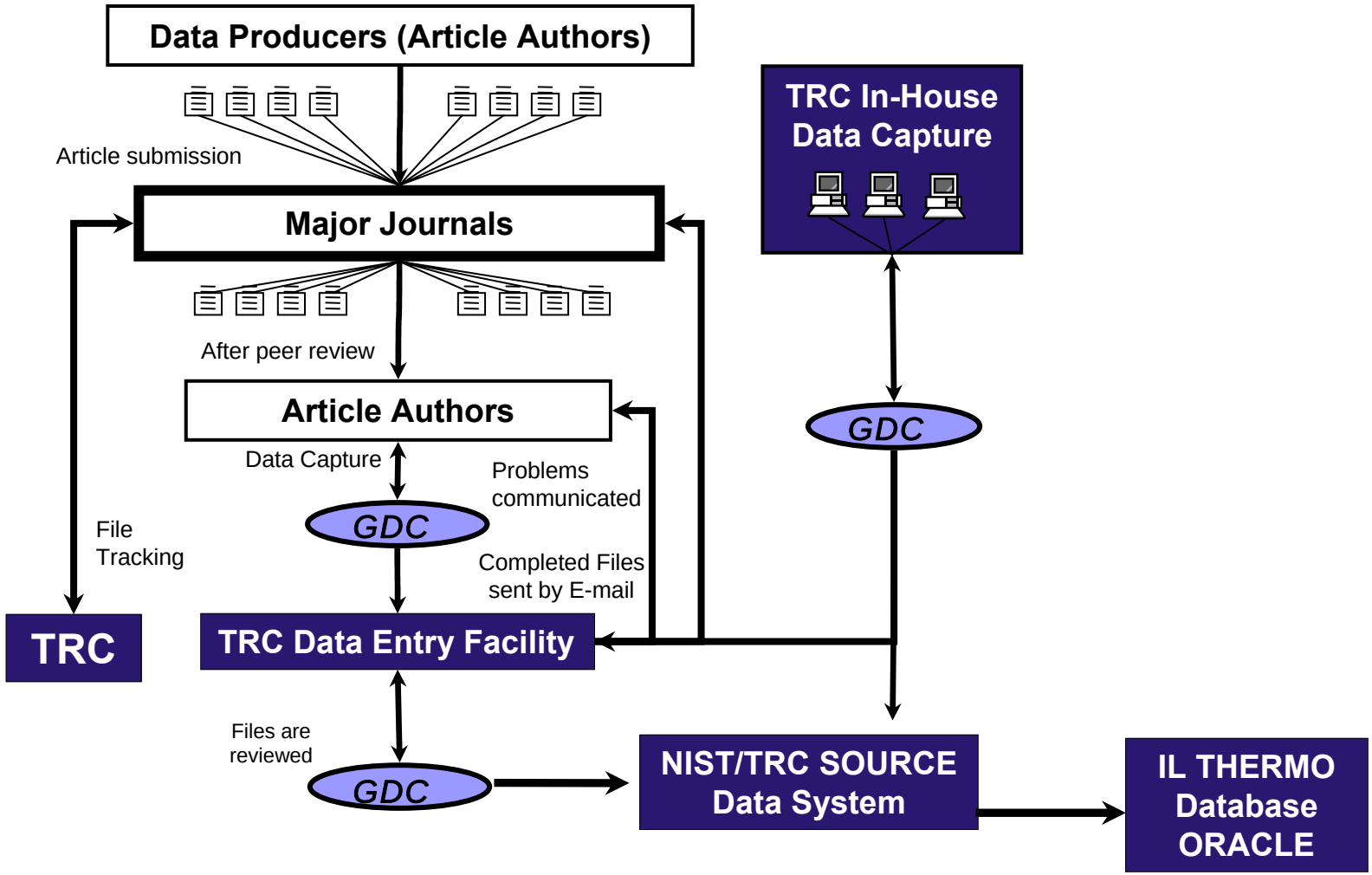
NIST/TRC

WEB

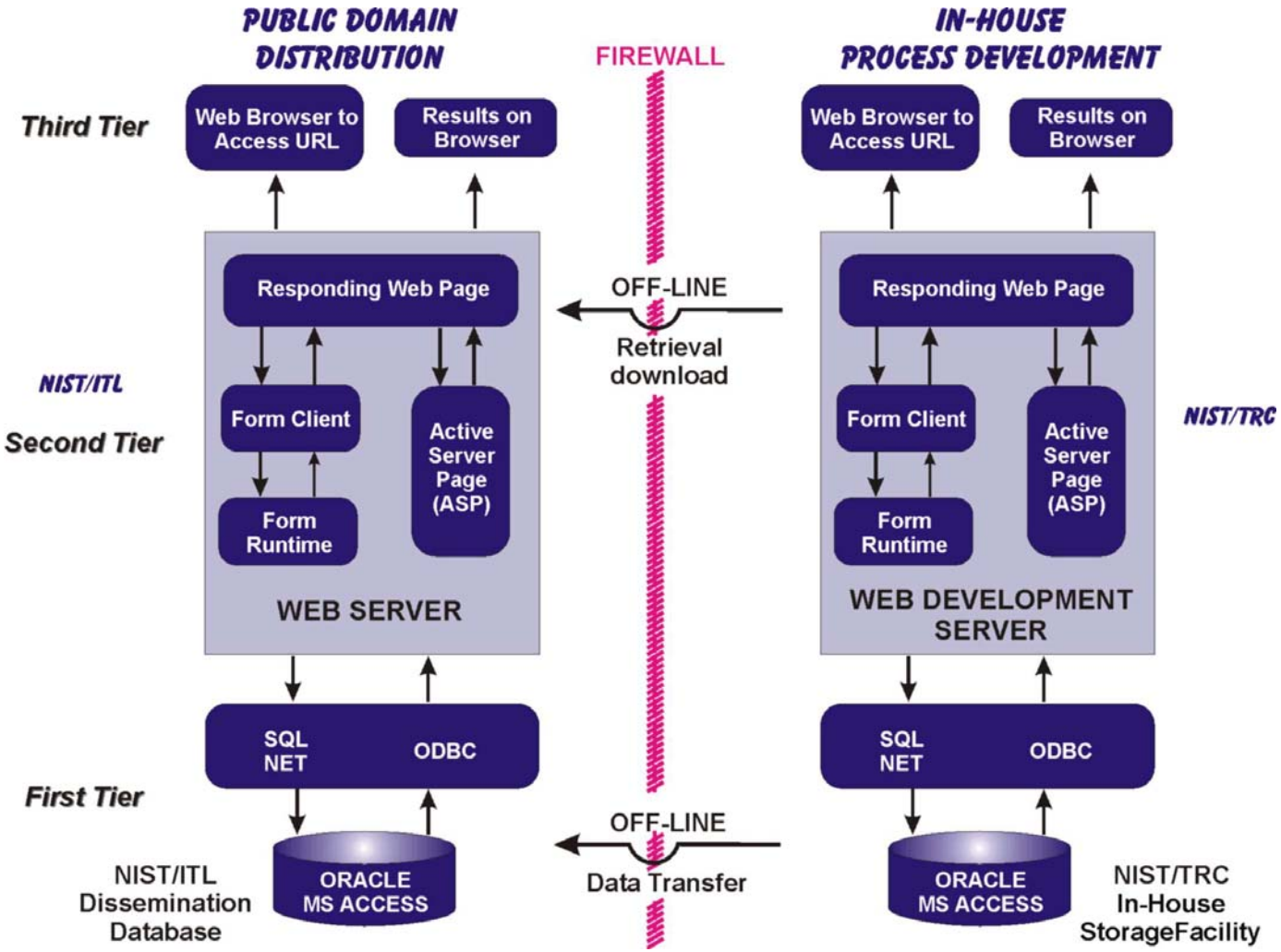
Applications

- AspenTech *(USA)*
- Virtual Materials Grp. *(Canada)*
- Nat'l Engineering Lab *(UK)*
- Fiz Chemie *(Germany)*

Industry: **DIPPR**


Data Producers (Article Authors)
Article submission
Major Journals
TRC In-House Data Capture
After peer review
Article Authors
GDC
Data Capture
Problems communicated
GDC
File Tracking
Completed Files sent by E-mail
TRC
TRC Data Entry Facility
Files are reviewed
GDC
NIST/TRC SOURCE Data System
IL THERMO Database ORACLE

Three-tier Web Database Process Flow



ILThermo

- **A key part of the IUPAC data retrieval system for ionic liquids**
- **Web-based relational database**
- **Addresses thermodynamic, thermochemical, thermophysical and chemical reaction data for ionic liquids**
- **Significant effort is proceeding to fully populate the database**

Search & Retrieval – Overview

Ions and ionic liquids

- *Ions and ionic liquids*
- *Compositional relations*
- *Ion structures*

Property data for pure ionic liquids

Property data for binary ionic liquids

Property data for ternary ionic liquids

Property data for reaction

Information displayed:

- *Ions*
- *Ion structures*
- *Ionic liquids*
- *Compositional relations*
- *Property data index*
- *Property/substance data summary*
- *Specific property data*
- *Specific measurement methods*
- *Specific measurement purpose*
- *Specific purity and purification*
- *Bibliography*

Search & Retrieval - Methods

- ***Search Methods***
  - ***Ions***
    - ***CASRN***
    - ***Formula***
    - ***Charge***
    - ***Names***
  - ***Ionic Liquids***
    - ***CASRN***
    - ***Formula***
    - ***Molecular mass***
    - ***Names***
  - ***Property***
  - ***Bibliography***
    - ***Author's name***
    - ***Journal title***
    - ***Article title***
    - ***Year of publication***

ILThermo Home Page

IUPAC Ionic Liquids Database - (ILThermo)

- IUPAC Ionic Liquids Database
- Thermodynamics Research Center
- National Institute of Standards and Technology

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

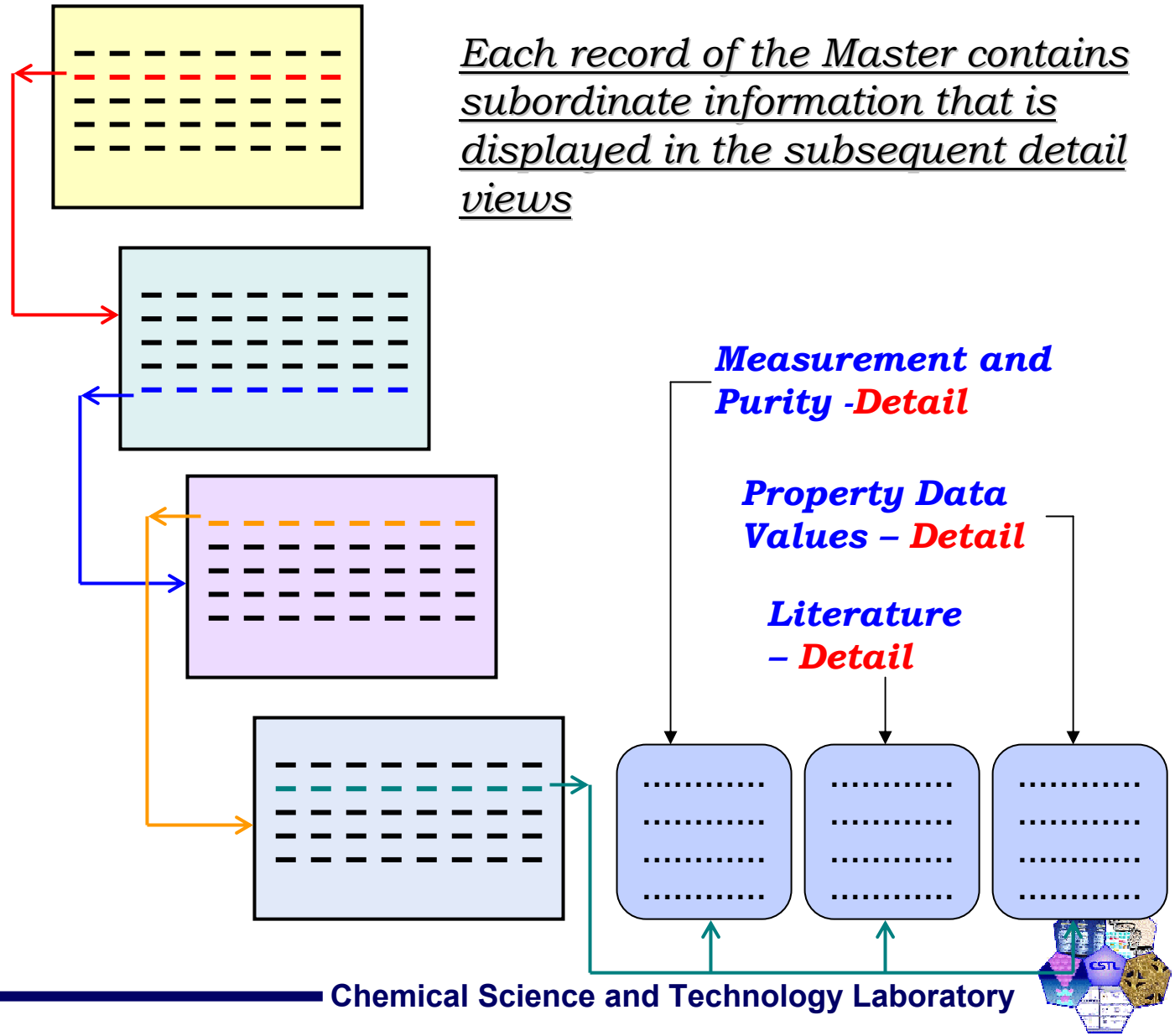
Multilevel Master/Detail Views for Ionic Liquids

List of Cation or Anion - Master

List of Ionic Liquids – Detail/Master

List of Properties – Detail/Master

List of Data Sets – Detail/Master



Each record of the Master contains subordinate information that is displayed in the subsequent detail views

Measurement and Purity -Detail

Property Data Values – Detail

Literature – Detail

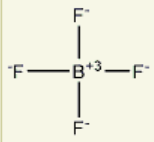
Search by Ion

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-);
○	[illegible]	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	

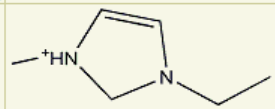
Ionic liquid(s) Containing the Ion - 14874705

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;

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

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.

Search by Reference

Search Property Data by Reference

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

Available Reference(s) Queried:

Select	Year_Pub.	Authors	Source
○	2002	Gu, Z.; Brennecke, J. F.	J. Chem. Eng. Data 47 , 339-345
○	2002	Krummen, M.; Wasserscheid, P.; Gmehling, J.	J. Chem. Eng. Data 47 , 1411-1417
○	2003	Domanska, U.; Marciniak, A.	J. Chem. Eng. Data 48 , 451-456
○	2003	Letcher, T. M.; Deenadayalu, N.	J. Chem. Thermodyn. 35 (1), 67-76
○	2003	Letcher, T. M.; Deenadayalu, N.; Soko, B.; Ramjugernath, D.; Naicker, P. K.	J. Chem. Eng. Data 48 , 904-907
○	2004	Arce, A.; Rodriguez, O.; Soto, A.	J. Chem. Eng. Data 49 , 514-517
○	2004	Domanska, U.; Mazurowska, L.	Fluid Phase Equilib. 221 , 73-82
○	2004	Fredlake, C. P.; Crosthwaite, J. M.; Hert, D. G.; Aki, S. N. V. K.; Brennecke, J. F.	J. Chem. Eng. Data 49 , 954-964
◉	2004	Kabo, G. J.; Blokhin, A. V.; Paulechka, Y. U.; Kabo, A. G.; Shymanovich, M. P.; Magee, J. W.	J. Chem. Eng. Data 49 , 453-461
○	2004	Kim, K.-S.; Shin, B.-K.; Ziegler, F.	Fluid Phase Equilib. 218 , 215-220
○	2004	Letcher, T. M.; Reddy, P.	Fluid Phase Equilib. 219 , 107-112
○	2004	Zhang, S.; Li, X.; Chen, H.; Wang, J.; Zhang, J.; Zhang, M.	J. Chem. Eng. Data 49 , 760-764
○	2005	Kumelan, J.; Kamps, A. P. -S.; Tuma, D.; Maurer, G.	Fluid Phase Equilib. 228-229 , 207-211
○	2005	Letcher, T. M.; Reddy, P.	J. Chem. Thermodyn. 37 , 415-421
○	2005	Van Valkenburg, M. E.; Vaughn, R. L.; Williams, M.; Wilkes, J. S.	Thermochim. Acta 425 , 181-188
○	2005	de Azevedo, R. G.; Esperanca, J. M. S. S.; Szydlowski, J.; Visak, Z. P.; Pires, P. F.; Guedes, H. J. R.; Rebelo, L. P. N.	J. Chem. Thermodyn. 37 , 888-899

Properties and Compounds Reported in ref - 2004 - Kabo, G. J.; Blokhin, A. V.; Paulechka, Y. U.; Kabo, A. G.; Shymanovich, M. P.; Magee, J. W.

Select	Property_Category	Description	Data_Points	CASRN	Chemical_Formula	Names
○	Heat Capacity	Heat capacity at saturation, J/(mol.K)	364	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
◉	Thermal Properties	(H-H0)/T, J/(K.mol)	49	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Phase Change Enthalpy	Enthalpy of transition or fusion, kJ/mol	1	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Thermal Properties	Entropy, J/(K.mol)	49	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Temperature	Triple point, K	1	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Volumetric Properties	Specific density, kg/m**3	10	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;

Selected Data Set (Property/Uncertainty - (H-H0)/T, J/(K.mol))

DataSet	Temperature, K	Property Value	Uncertainty
1	5	0.24603	0.0254
1	10	1.92979	0.052
1	15	5.68128	0.1014
1	20	10.8338	0.15
1	25	16.737	0.191
1	30	22.8648	0.216
1	35	28.9177	0.249
1	40	34.7628	0.274
1	45	40.3335	0.299
1	50	45.6132	0.333
1	60	55.2996	0.374
1	70	63.9965	0.424
1	80	71.9202	0.457
1	90	79.2452	0.515
1	100	86.1379	0.58
1	110	92.7064	0.58
1	120	98.9422	0.58
1	130	105.012	0.58
1	140	110.915	0.67
1	150	116.818	0.67
1	160	122.555	0.67
1	170	128.292	0.75
1	180	134.029	0.75
1	190	139.766	0.75
1	200	145.503	0.75
1	210	151.24	0.831
1	220	157.06	0.831
1	230	162.797	0.831
1	240	168.451	0.915
1	250	174.188	0.915
1	260	179.842	0.915
1	270	185.579	0.915
1	280	191.316	0.998
1	283.51	193.311	0.998

Search by Reference

Search Property Data by Reference

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

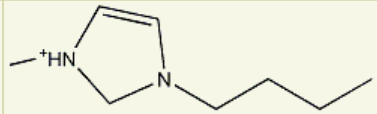
Available Reference(s) Queried:

Select	Year_Pub.	Authors	Source
○	2002	Gu, Z.; Brennecke, J. F.	J. Chem. Eng. Data 47 , 339-345
○	2002	Krummen, M.; Wasserscheid, P.; Gmehling, J.	J. Chem. Eng. Data 47 , 1411-1417
○	2003	Domanska, U.; Marciniak, A.	J. Chem. Eng. Data 48 , 451-456
○	2003	Letcher, T. M.; Deenadayalu, N.	J. Chem. Thermodyn. 35 (1), 67-76
○	2003	Letcher, T. M.; Deenadayalu, N.; Soko, B.; Ramjugernath, D.; Naicker, P. K.	J. Chem. Eng. Data 48 , 904-907
○	2004	Arce, A.; Rodriguez, O.; Soto, A.	J. Chem. Eng. Data 49 , 514-517
○	2004	Domanska, U.; Mazurowska, L.	Fluid Phase Equilib. 221 , 73-82
○	2004	Fredlake, C. P.; Crosthwaite, J. M.; Hert, D. G.; Aki, S. N. V. K.; Brennecke, J. F.	J. Chem. Eng. Data 49 , 954-964
◉	2004	Kabo, G. J.; Blokhin, A. V.; Paulechka, Y. U.; Kabo, A. G.; Shymanovich, M. P.; Magee, J. W.	J. Chem. Eng. Data 49 , 453-461
○	2004	Kim, K.-S.; Shin, B.-K.; Ziegler, F.	Fluid Phase Equilib. 218 , 215-220
○	2004	Letcher, T. M.; Reddy, P.	Fluid Phase Equilib. 219 , 107-112
○	2004	Zhang, S.; Li, X.; Chen, H.; Wang, J.; Zhang, J.; Zhang, M.	J. Chem. Eng. Data 49 , 760-764
○	2005	Kumelan, J.; Kamps, A. P. -S.; Tuma, D.; Maurer, G.	Fluid Phase Equilib. 228-229 , 207-211
○	2005	Letcher, T. M.; Reddy, P.	J. Chem. Thermodyn. 37 , 415-421
○	2005	Van Valkenburg, M. E.; Vaughn, R. L.; Williams, M.; Wilkes, J. S.	Thermochim. Acta 425 , 181-188
○	2005	de Azevedo, R. G.; Esperanca, J. M. S. S.; Szydlowski, J.; Visak, Z. P.; Pires, P. F.; Guedes, H. J. R.; Rebelo, L. P. N.	J. Chem. Thermodyn. 37 , 888-899

Properties and Compounds Reported in ref - 2004 - Kabo, G. J.; Blokhin, A. V.; Paulechka, Y. U.; Kabo, A. G.; Shymanovich, M. P.; Magee, J. W.

Select	Property_Category	Description	Data_Points	CASRN	Chemical_Formula	Names
◉	Heat Capacity	Heat capacity at saturation, J/(mol.K)	364	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Thermal Properties	(H-H0)/T, J/(K.mol)	49	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Phase Change Enthalpy	Enthalpy of transition or fusion, kJ/mol	1	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Thermal Properties	Entropy, J/(K.mol)	49	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Temperature	Triple point, K	1	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;
○	Volumetric Properties	Specific density, kg/m**3	10	174501645	C8H15F6N2P	1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;

Ions constituting the ionic liquid - 174501645

CASRN	Chemical_Formula	Charge	Names	Image
16919189	F6P	-1	Hexafluorophosphate; Hexafluorophosphate ion; Hexafluorophosphate(1-); Hexafluorophosphate(1-) ion; Phosphate(1-), hexafluoro- ;	
80432082	C8H15N2	1	1-Butyl-3-methylimidazolium; 1H-Imidazolium, 1-butyl-3-methyl- ;	

Data Summary

Property: Heat capacity at saturation, J/(mol.K)

Compound: Name - 1-N-butyl-3-methylimidazolium hexafluorophosphate; 1-butyl-3-methylimidazolium hexaflourophosphate; 1-butyl-3-methylimidazolium hexafluorophosphate; 1H-imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-) ;

CASRN - 174501645 Formula - C8H15F6N2P

Total Data Points: 364

References: Year and Authors - - 2004 ; Kabo, G. J.; Blokhin, A. V.; Paulechka, Y. U.; Kabo, A. G.; Shymanovich, M. P.; Magee, J. W.

Source - J. Chem. Eng. Data 49 , 453-461

Title - Thermodynamic Properties of 1-Butyl-3-methylimidazolium Hexafluorophosphate in the Condensed State

Abstract - Thermodynamic functions for 1-butyl-3-methylimidazolium hexafluorophosphate ([C4mim][PF6]) were reported in a range of temperatures from (5 to 550) K, based on new measurements by calorimetry. Heat capacities of the crystal, glass and liquid phases for [C4mim][PF6] were measured with a pair of calorimeters. A vacuum-jacketed adiabatic calorimeter was used at temperatures between (5 and 310) K and a triple-heat bridge scanning calorimeter was used from (300 to 550) K. With the adiabatic calorimeter, both the fusion temperature (283.51 K) and enthalpy (19.60 kJ.mol-1) and the glass transition temperature (190.6 K) were observed. The purity of the [C4mim][PF6] sample was determined to be 99.56 mol % by a fractional melting analysis. Densities of the liquid were measured in a range of temperatures from (298 to 353) K with a pycnometer equipped with a capillary neck. An unexpected endothermal transition, with a very small enthalpy change of 0.25 J¿g-1 (0.071 kJ¿mol-1) was observed in a range of temperatures from (394 to 412) K. Heat capacity jumps were determined at the glass transition, 81.6 J.K-1.mol-1, and fusion, 44.8 J.K-1.mol-1, and the observed entropy change at fusion is 69.23 J.K-1.mol-1.

Keywords - heat capacity, thermodynamic functions, 1-butyl-3-methylimidazolium hexafluorophosphate

References and Data Sets

Select	Data Type	Data Set	Variable1	Variable2	Phase1	Phase2	Phase3
◉	One Variable	1	Temperature, K		Crystal	Gas	
○	One Variable	2	Temperature, K		Liquid	Gas	
○	One Variable	3	Temperature, K		Glass	Gas	
○	One Variable	4	Temperature, K		Crystal	Gas	
○	One Variable	5	Temperature, K		Liquid	Gas	
○	One Variable	6	Temperature, K		Glass	Gas	

Purity and Measurement

Source: Commercial source
Initial Purity: Not stated
Purification: Dried by heating in a vacuum
Final Purity: 99.56 mol %
Purity Analysis: Thermal analysis using a calorimeter

Measurement Purpose: Direct observation
Measurement Method: Small (less than 1 g) adiabatic calorimetry

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

Previous 1-25 of 137 Next 25

DataSet	Temperature, K	Property Value	Uncertainty
1	5.13	1.06508	0.033
1	5.41	1.23054	0.036
1	5.67	1.40515	0.038
1	5.97	1.62548	0.042
1	6.29	1.92729	0.046
1	6.6	2.26403	0.051
1	6.91	2.56585	0.055
1	7.23	2.99404	0.06
1	7.58	3.43471	0.066
1	7.92	3.84794	0.072
1	8.28	4.39503	0.079
1	8.66	4.98951	0.0865
1	9.07	5.73948	0.0956
1	9.49	6.47864	0.1039
1	9.92	7.35166	0.1139
1	10.35	8.19474	0.1239
1	10.75	9.00457	0.133
1	11.18	10.0439	0.141
1	11.74	11.2911	0.158
1	12.32	12.5715	0.166
1	12.92	14.0847	0.183
1	13.56	15.7227	0.2
1	14.2	17.2608	0.216
1	14.85	19.0568	0.233
1	15.51	20.7612	0.241

Previous 1-25 of 137 Next 25

Statistics for *IL Thermo* August 4, 2005

- Last populated August 4, 2005
- Collection consists of pure ionic liquids, binary systems containing ionic liquids, and ternary systems containing ionic liquids.
- Statistical data with break out by type of system:
  (1) Pure component properties -- 1048 data points
- (2) Binary systems containing ionic liquids -- 2602 data points
- (3) Ternary systems containing ionic liquids -- 1145 data points
- (4) Overall, those data records cover:
- (a) 19 ionic liquids that are composed of 10 ions,
- (b) 137 binary systems
- (c) 50 ternary systems
- (d) 50 properties
- (e) 32 articles (JCED - 20, JCT- 4, Fluid Phase Equilib. - 7, and Thermochim Act - 1)
- (f) 4795 total data points

2nd Task Group Meeting

Beijing International Convention Center
Beijing, China August 12, 2005

- Present: Marcelle Gaune-Escard, Michael Frenkel, Joseph Magee, Kenneth Marsh, Kenneth Seddon, Slobodan Gadzuric (observer)
- Structure and information input methods for ILThermo
  - Guided Data Capture (GDC) software
  - ThermoML IUPAC standard for storage and exchange of data
- Search and retrieval from ILThermo
- Public release of ILThermo – will follow internal review procedures
- Distributed access system – a desirable long-range goal with various types of data being independently managed
- Coverage would include synthesis, catalysis, structure, manufacturing, modeling as well as physical and chemical property data with their associated uncertainties
- Avoid duplication of effort – populate ILThermo with high-temperature molten salt data and coordinate efforts with other database developers

MINUTES OF SECOND IONIC LIQUIDS DATABASE MEETING
(#2003-020-2-100)

IUPAC GENERAL ASSEMBLY
BEIJING INTERNATIONAL CONVENTION CENTER
BEIJING, CHINA, 12TH AUGUST 2005

PRESENT

Kenneth R. Seddon (Chair), Kenneth N. Marsh, Marcelle Gaune-Escard, Joseph W. Magee, Michael Frenkel (members) and Slobodan Gadzuric (observer)

OPENING REMARKS

The Chair welcomed all in attendance. Apologies were offered from those unable to attend. Introductions were made. The Task Group expressed their thanks to IUPAC-GA organizers for hosting the meeting and logistical support for the IL database task group meeting.

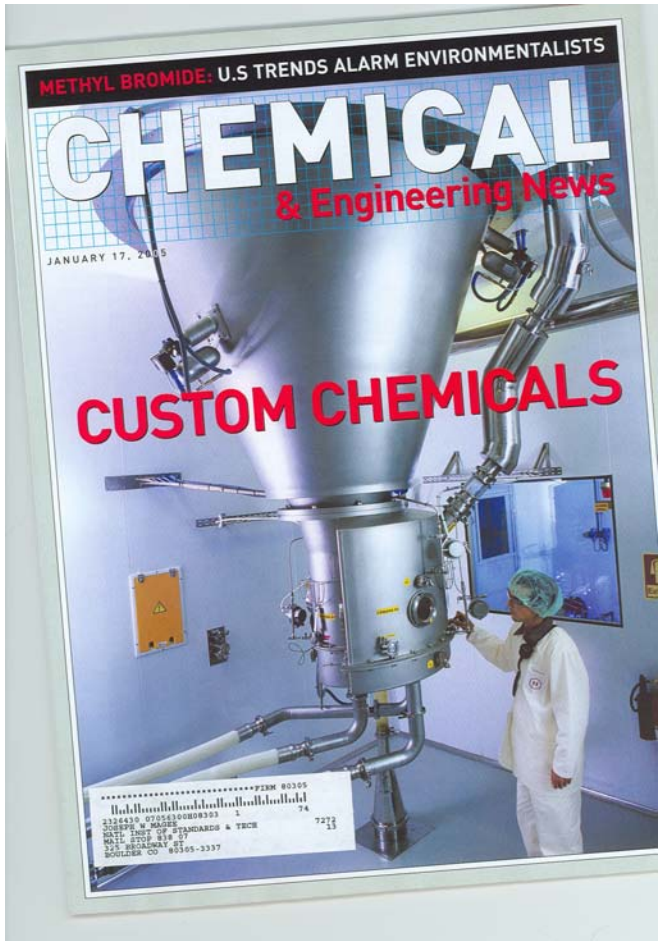
DATABASE PROJECT UPDATE

Drs. Magee and Frenkel of NIST gave a detailed presentation on the structure and input methods for the recently developed database, called ILThermo. The discussion began with a review of the background and genesis of the project, as follows. Progress in utilizing ionic liquids had been hampered by the lack of an open-access, public domain, comprehensive data retrieval system scoped to cover information pertaining to ionic liquids. Development of such a database infrastructure encompasses a number of complex issues related to data submission, processing, mining, quality control, management, critical evaluation, and dissemination. It is also obvious that such a system should provide coverage for various types of data such as synthesis, catalysis, structure, manufacturing, modeling as well as thermophysical and thermochemical property data. A broad-based international effort would be needed to develop such an information system. Thus the present IUPAC project (2003-020-2-100) *Ionic Liquids Database* (K. R. Seddon (Task Group Chair), A. Burgess, M. Frenkel, M. Gaune-Escard, A. Heintz, J. W. Magee, K. N. Marsh, R. Sheldon (members)) was formed to address this need.

On January 26, 2004 the task group met at the Technical University of Delft (Delft, Netherlands) to decide on a common vision for the project and to divide the data collection effort amongst the participants. A second meeting had been deemed necessary when a preliminary version of the database was ready for testing.

The discussion then turned to the preliminary version of the ionic liquids database and exploring future tasks. In particular, the relationship between the primary NIST molten salt database and the new ionic liquids database was explored. The enormous number of publications concerning ionic liquids in 2004 (approx. 2500 papers) and the foreseeable growth expected in the future requires proper data collection, storage and retrieval from searchable electronic archives. The new database will be significantly more inclusive than NIST Standard Reference Database 27: NIST Molten Salts Database that provides molten state properties (density, surface tension, viscosity, electrical conductance) for 320 inorganic salts and 4,000 mixtures.

Letter to Editor of *C&EN*



Ionic liquid database

MY COLLEAGUES AND I APPRECIATE your very fine article on organic synthesis with ionic liquids (C&EN, Nov. 8, 2004, page 44). The article covered the subject with a depth that is rarely seen.

I strongly support the statement in the article that "it is important to develop a good database of all the information available on ionic liquids. Unless we have all this information, the growth will be limited to a few sectors."

I can also offer some information about efforts that directly address the expressed need. In 2003, an international effort was launched through the International Union of Pure & Applied Chemistry to meet this important need. The IUPAC project (Number 2003-020-2-100) is titled "Ionic Liquids Database." The task group chair is Kenneth R. Seddon of Queens University, Belfast, Northern Ireland. Task group members, representing industry, academia, and government, are Andrew Burgess, Michael Frenkel, Marcelle Gaune-Escard, Andreas Heintz, Joseph Magee, Kenneth Marsh, and Roger Sheldon.

The project's objective is to address the need for an open-access, public-domain data storage system scoped to cover information pertaining to ionic liquids. The vision for this project is to create a distributed-access data retrieval system for ionic liquids and their mixtures that encompasses chemical structure, solvent properties, ionic liquids use in synthesis, reviews, reactions and catalysis, manufacturer information, benchmark properties and models, and thermophysical and thermochemical data.

In January of 2004, the task group met in Delft, the Netherlands, to develop a shared vision and to divide the data collection effort among the participants. More information on this project is available from IUPAC at http://www.iupac.org/projects/2003/2003-020-2-100.html.

JOSEPH MAGEE
Boulder, Colo.

Update to IUPAC Project Web Site

assessment of overall uncertainties of the data, and will facilitate reports of recommended values. Software has been prepared that will automatically extract ionic liquids data from the SOURCE system. Making this unique tool for automatic data evaluation available to this project will streamline the assessment and compilation of thermodynamic, thermochemical and transport properties of ionic liquids.

When each subgroup's data has been compiled into agreed-upon formats, the parts will be combined into a beta version of the entire database. It then will be tested by a wide range of users, whose comments will be solicited to improve the product. When the improvements have been implemented and tested, IUPAC Ionic Liquids Database version 1.0 will be released to the public. NIST will provide web space with a single-entry point for all users of this database, and provide the tools to measure usage and compile a monthly statistical report for the website. As part of an ongoing commitment, NIST will maintain this database on a NIST server and update its holdings on a regular basis. Our long-range operating plan, built upon continuous exchange and cooperation with both data generators and users, will streamline the process of adding new results and making further improvements better to serve the needs of the international chemistry community.

Progress:
On January 26, 2004 the task group met at the Technical University of Delft (Delft, Netherlands) to discuss a common vision for the project and to divide the data collection effort amongst the participants. As an example, M. Frenkel and J. Magee (leaders of the NIST team) were assigned responsibility to develop (1) a Web outlet for the system and (2) a storage and retrieval system for thermophysical and thermochemical property data of ionic liquids.

Since the first Task Group meeting, there has been significant progress to report. To date *(May 2005)*, the NIST team has modified the Thermodynamics Research Center's SOURCE database and the Guided Data Capture application to facilitate the storage and retrieval of ionic liquids property data and have created a web-based properties retrieval system by using an Oracle Java Application Development Frame. This system has been successfully deployed on an Apache Jakarta Tomcat 5 Application Server implementing selected multi-tier architecture of the Web Oracle dissemination infrastructure. Presently, search functionality within the properties database is undergoing rigorous internal testing. An external launch of the property database,

named ILTHERMO, is anticipated for December, 2005. Also, other task group members are preparing their specific data holdings in anticipation that they will be interfaced with the system Web outlet.

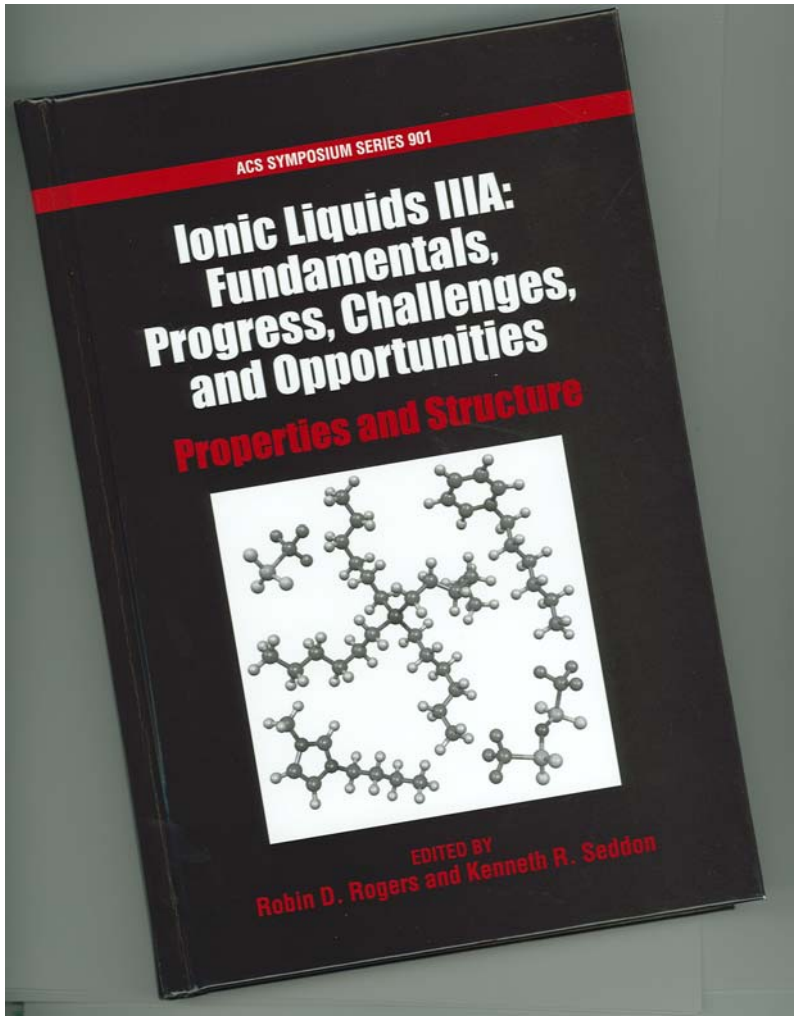
Task group members will report their progress on their individual assignments and will discuss building the linkages within the data retrieval system infrastructure at a meeting scheduled in Beijing to be held in conjunction with the 40th IUPAC Congress.

Last update: 31 May 2005

<project announcement to be published in *Chem. Int.*>

If you want to update this information, contact us by e-mail
Do not forget to include the Project Number, your name and relation with that project

Chapter in ACS Symposium Series 901



Chapter 12

Physical Property Measurements and a Comprehensive Data Retrieval System for Ionic Liquids

Joseph W. Magee[1], Gennady J. Kabo[2], and Michael Frenkel[3]

[1]Experimental Properties of Fluids Group and [3]Thermodynamics Research Center, Physical and Chemical Properties Division, National Institute of Standards and Technology, MS 838.07, 325 Broadway, Boulder, CO 80305–3328
[2]Chemistry Department, Belarusian State University, Leningradskaya 14, Minsk 220050, Belarus

NIST has initiated a collaborative project to provide key physical properties of a subset of ionic liquids that represent a selection of cations, anions and substituent chemical groups. NIST is collaborating with IUPAC task groups to establish standardized systems and to develop a comprehensive data retrieval system for ionic liquids.

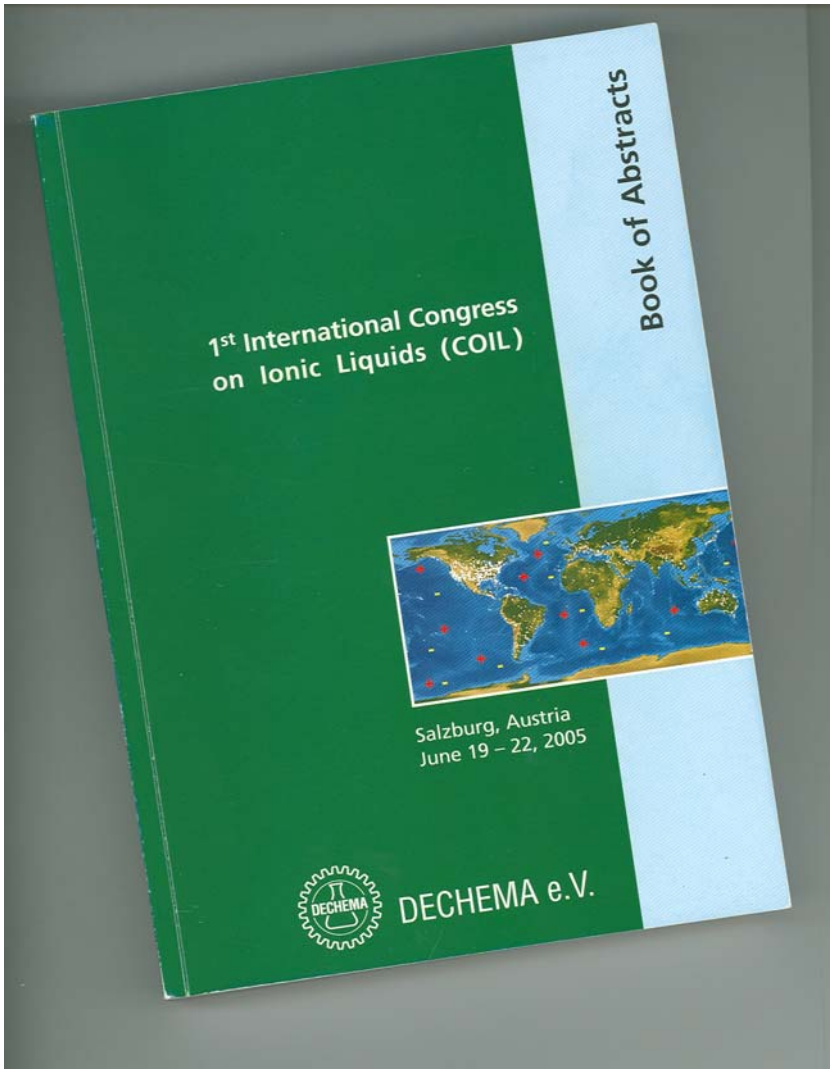
By a judicious choice of its cation, anion, and substituent chemical groups, it is possible to tailor the physical properties of room-temperature ionic liquids (RTIL). Various research groups have reported physical properties for RTIL over ranges of temperature and pressure, including melting points, densities, viscosities, solubilities, liquid-liquid phase equilibria, heat capacities, etc. A broad review of this subject has recently become available (*1*). To date, reports of some physical properties such as thermal conductivity are quite scarce. Benchmark physical properties of high accuracy are scarcer still. For these reasons, NIST has initiated a project to provide key physical properties of a subset of RTIL that represent a selection of cations, anions and substituent chemical groups. An IUPAC task group has been formed to address these concerns and a recognized need for relevant standardized systems.

As identified at a NATO Workshop in Heraklion, Greece, a verified, web-based, public-access database of RTIL properties data is an important need of the ionic liquids community. NIST has begun to address this need by evaluating published measurements on RTIL and capturing the data into a comprehensive data retrieval system known as SOURCE. SOURCE is an archival system that presently captures more than 120 properties and contains 1.3 million data points on 17,000 different substances and 12,000 mixtures. The ionic liquids database will be built by using a record structure similar to SOURCE and maintained by the Oracle (*2*) relational database management system. Guided Data Capture (GDC) software will be used to speed collection of new experimental data directly from experimentalists. A second IUPAC task group has been formed to address the neeed for a comprehensive data retrieval system for RTIL.

Physical Properties

The Physical and Chemical Properties Division of NIST has developed experimental capabilities for wide-ranging, high-accuracy fluid physical properties measurements. Considering the properties types and their ranges, NIST's facilities are among the most comprehensive available in the world. It has performed experimental research on the thermodynamic and transport properties of industrially important fluids and fluid mixtures covering temperatures from 5 K to over 800 K at pressures to 70 MPa, over the full range of compositions for mixtures. It uses specially designed apparatus to measure density, heat capacity, speed of sound, phase equilibrium behavior, interfacial tension, viscosity, and thermal conductivity. Over a period of more than 40 years, the Division has used these apparatus to measure properties of cryogenic gases, natural gases, alternatives to CFC refrigerants, liquefied fuels, and aqueous systems. A program has been initiated to measure, within established limits of uncertainities, key physical properties of ionic liquids.

1st International Congress on Ionic Liquids



Comprehensive Data Retrieval System for Ionic Liquids

Joseph W. Magee and Jason A. Widegren
Experimental Properties of Fluids Group
Michael Frenkel, Qian Dong, Chris Muzny, Robert D. Chirico and Vladimir V. Diky
Thermodynamics Research Center
Physical and Chemical Properties Division
National Institute of Standards and Technology
Boulder, Colorado USA

1st International Congress on Ionic Liquids (COIL)
Salzburg, Austria
June 19-22, 2005

Chemical Science and Technology Laboratory