

## ILThermo Version 2.0: Archival Storage and Retrieval of Thermophysical Properties for Ionic Liquids

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Originally developed under the auspices of IUPAC (Project 2003-020-2-100), ILThermo [1] (<http://ilthermo.boulder.nist.gov/>) is an archival database of experimental thermophysical properties of ionic liquids and mixtures that contain them. The original version had its public release in 2006. In 2013, Version 2.0 [2] was released by the Thermodynamics Research Center of the NIST Material Measurement Laboratory, Applied Chemicals and Materials Division. ILThermo is a web-based open-access database that provide up-to-date information on publications of the results of experimental studies of ionic liquids, including numerical values of thermophysical and thermochemical properties, chemical structures, measurement methods, sample purity, critically evaluated uncertainty of property values, as well as other significant measurement details. In the intervening nine years since its public release (July, 2006), NIST has continued to populate ILThermo with information derived from recently published articles. While ILThermo's data population has doubled twice, at the same time this work has seen significant challenges. The challenges that are central to this effort include: high volume of relevant articles; wide dispersion of published articles; wide variety of possible cations and anions; inconsistent compound nomenclature and abbreviations; and, poor availability of compound registry numbers. We describe how those challenges were addressed and solutions that were developed. In addition, NIST has seized upon new opportunities to broaden the scope and functionality of on-demand data evaluation that is feasible within the ionic liquids archive. Such on-demand evaluations are carried out with the application NIST ThermoData Engine (TDE), which is a software implementation of the concept of dynamic data evaluation. We describe key opportunities that include experiment planning and product design for ionic liquids. Planning tools would be considered most useful when they help experimentalists prioritize their measurements on ionic liquids. Such outcomes of planning are meaningful only if the underlying evaluation for a given property takes into consideration their uncertainties, their measurement ranges, and essentially all published values. Experiment planning tools will answer queries such as What should I measure that will have a significant impact? In addition, process engineers need product design tools that help identify candidate ionic liquids that have a set of desired properties. Product design tools will answer queries such as Which ionic liquid has the right thermophysical properties for my process application? We discuss NIST's approach to these research opportunities, beginning with development and a recent release of TDE software and leading to future developments of TDE. Research will be necessary to extend TDE, presently applicable to molecular compounds, to ionic liquids and mixtures that contain them.

### References

- [1] Q. Dong, C. D. Muzny, A. Kazakov, V. Diky, J. W. Magee, J. A. Widegren, R. D. Chirico, K. N. Marsh, and M. Frenkel, *J. Chem. Eng. Data* 52, 1151-1159 (2007).
- [2] A. Kazakov, J.W. Magee, R.D. Chirico, V. Diky, C.D. Muzny, K. Kroenlein and M. Frenkel "NIST Standard Reference Database 147: NIST Ionic Liquids Database - (ILThermo)", Version 2.0, National Institute of Standards and Technology, Gaithersburg MD, 20899, <http://ilthermo.boulder.nist.gov> .