

## ThermoML: New IUPAC Standard for Thermodynamic Data Communications

*The NIST Thermodynamics Research Center has played a key role in the developing and establishing international standard for XML by leading an IUPAC effort titled "XML-based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture". This project addresses the interoperability problem between the formats and structures of thermodynamic data files and required input/output structures for the software applications.*

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Thermodynamic property data represent a key resource for development and improvement of all chemical process technologies. However, rapid growth in the number of custom-designed software tools for engineering applications has created an interoperability problem between the formats and structures of thermodynamic data files and required input/output structures for the software applications. Establishment of efficient means for communication of thermodynamic data is absolutely critical for provision of solutions to such technological challenges as elimination of data processing redundancies and data collection process duplication, creation of comprehensive data storage facilities, and rapid data propagation from measurement to data-management system and from data-management system to engineering application. Taking into account the diversity of thermodynamic data and numerous methods of their reporting and presentation, standardization of thermodynamic data communications is very complex.



Since 2002, the NIST Thermodynamics Research Center of the Physical and Chemical Properties Division has played a key role in the development and establishment of the interna-

tional standard, leading the efforts of the Task Group for IUPAC project 2002-055-3-024, "XML-based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture". This project has recently been successfully completed with the establishment of the new IUPAC standard for thermodynamic data communications, ThermoML. The full description of ThermoML was published in the March issue of Pure and Applied Chemistry (Vol. 78, No. 3, pp. 541–612, 2006), and the ThermoML namespace has been established on the IUPAC Web site.

The role of ThermoML in thermodynamic data communications is reflected in making a significant impact for development of efficient chemical engineering applications, including chemical process design, providing new capabilities for data delivery from 'data producers' to 'data users', establishing software 'tools' designed to improve the quality of published experimental data, as well as new mechanisms for development of a variety of data products serving the scientific and engineering communities. The development of ThermoML and the software infrastructure supporting it has led to a unique cooperation between five major journals in the field (Journal of Chemical and Engineering Data, The Journal of Chemical Thermodynamics, Fluid Phase Equilibria, Thermochemica Acta, and International Journal of Thermophysics), three scientific publishers (ACS, Elsevier, and Springer), NIST, IUPAC, and leading chemical process design companies.

Recently, the symposium, "ThermoML: Purpose, Structure, and Applications" was organized by the American Chemical Society (ACS) at its Spring 2006 National Meeting in Atlanta, Georgia. Speakers from the United States, Canada, UK, Germany, Netherlands, and New Zealand represented all components of the global data delivery process based on ThermoML. The announcement of ThermoML as a new IUPAC standard was made on March 27, 2006 by IUPAC President Prof. Bryan R. Henry during a special "ThermoML" reception co-sponsored by IUPAC, NIST, FizChemie Berlin (Germany), and Elsevier (Netherlands).

Future plans include expansion of the ThermoML for thermodynamic and transport properties of biomaterials.

### **International Project Team:**

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*M. Frenkel opens the ACS ThermoML Symposium. Honorable guests (right to left): Daniel Friend, Acting Chief of the Physical and Chemical Properties Division, NIST, Bryan R. Henry, IUPAC President (University of Guelph, Canada), and Catherine T. Hunt, President-Elect of ACS (Rohm and Haas Company).*

