XML-Based IUPAC Standard for Experimental, Predicted, and Critically Evaluated Thermodynamic Property Data Storage and Capture (ThermoML) (IUPAC Recommendations 2006)

Michael Frenkel, Robert D. Chiroco, Vladimir Diky, Qian Dong, Kenneth N. Marsh, John H. Dymond, William A. Wakeham, Stephen E. Stein, Erich Königsberger, and Anthony R.H. Goodwin

Pure and Applied Chemistry
Vol. 78, No. 3, pp. 541-612 (2006)
doi:10.1351/pac200678030541

ThermoML is an Extensible Markup Language (XML)-based new IUPAC standard for storage and exchange of experimental, predicted, and critically evaluated thermophysical and thermochemical property data. The basic principles, scope, and description of all structural elements of ThermoML are discussed. ThermoML covers essentially all thermodynamic and transport property data (more than 120 properties) for pure compounds, multicomponent mixtures, and chemical reactions (including change-of-state and equilibrium reactions). Representations of all quantities related to the expression of uncertainty in ThermoML conform to the *Guide to the Expression of Uncertainty in Measurement*. The ThermoMLEquation schema for representation of fitted equations with ThermoML is also described and provided as supporting information together with specific formulations for several equations commonly used in the representation of thermodynamic and thermophysical properties. The role of ThermoML in global data communication processes is discussed. The text of a variety of data files (use cases) illustrating the ThermoML format for pure compounds, mixtures, and chemical reactions, as well as the complete ThermoML schema text, are provided as supporting information.

www.iupac.org/publications/pac/2006/7803/7803x0541.html

Letters in Support of the ThermoML Standard

In a linking agreement between Elsevier and the Thermodynamic Research Center at NIST (USA), the ThermoML standard is used to make freely available thermochemical and physical property data connected to published articles. It concerns articles from *The Journal of Chemical Thermodynamics* (since 2004), *Fluid Phase Equilibria*, and *Thermochimica Acta* (since 2005). Thanks to the ThermoML standard, this data is now available in an as universal-as-possible format, to scientists and engineers in industry and university laboratories. A link to the ThermoML record is available with the journal article on <ScienceDirect.com>, while the respective journal article in which the data was reported can be found following a link on the data record. The editors of the journals and Elsevier consider this a major addition to the published content, and so are our authors who are pleased and eager to submit.

Michiel Thijssen <m.thijssen@elsevier.com>
Publishing Editor,
Elsevier B.V., Amsterdam

ThermoML will continue to have a positive impact on data activities, including scientific publishing (it is already used by five major journals), development of properties databases, and development of tools to correlate or to accurately predict thermodynamic quantities. I would anticipate that the proposed IUPAC standard will have an important role in the sharing of data between research groups as well as the storage and retrieval of such data. In addition, the standard addresses uncertainties of the data in a way that is consistent with the comprehensive reference document *Guide to the Expression of Uncertainty in Measurement* published by the International Organization for Standardization. The power of this concept lies in the fact that a complete knowledge of a physical quantity consists of a numerical value, its units, its uncertainty, and its provenance. This concept can help to create information and knowledge management systems that could carry the field of thermodynamics to the next level of intelligent predictive tools.

Joseph Magee <joe.magee@nist.gov>
National Institute of Standards and Technology, Boulder, Colorado USA