XML-Based IUPAC Standard for Experimental and Critically Evaluated Thermodynamic Property Data Storage and Capture

IUPAC has approved a project to develop an XML-based IUPAC standard for thermodynamic data communications as one of the activities of the Committee on Printed and Electronic Publication. Thermophysical and thermochemical property data represent a key foundation for development and improvement of all chemical process technologies. These data are also critical for support of fundamental research in physics, chemistry, biology, and material science.

The unprecedented growth in the number of custom-designed software tools for various engineering applications has created an interoperability problem between the formats and the structures of the thermodynamic data files and required input/output structures of different software products. This problem is reflected in the extremely time- and resource-consuming efforts required to collect the data within a particular data management environment using numerous data sources of different types. Within the last 20 years this problem has become a major obstacle to developing efficient process-design software tools, requiring generation of extensive thermophysical and thermochemical property data packages. The major objective of this project is to provide a practical solution to the problem by establishing an international standard for thermophysical/thermochemical data storage and exchange.

A standardized XML-based dictionary will provide the most powerful, interoperability solution for interpretation and use of thermodynamic data. Such a dictionary has to be able to describe the complete set of thermophysical and thermochemical properties (more than 120), their uncertainties, and related metadata. XML (Extensible Markup Language) avoids common pitfalls in language design: it is extensible and platform-independent. Since XML files are essentially textual files, they can be easily analyzed without the use of specific customized software products and can be read by a variety of text editors. The XML-based structure will represent a balanced combination of hierarchical and relational elements. It will explicitly incorporate structural elements related to basic principles of phenomenological thermodynamics: thermochemical and thermophysical (equilibrium and transport) properties, state variables, system constraints, phases, and units. The structural features of the metadata records will ensure unambiguous interpretation of numerical data as well as data-quality control based on the Gibbs Phase Rule. The developed dictionary will provide elements for storage and exchange of experimental, critically evaluated, and predicted data. The schema will have provisions for the expressions of various measures of the thermodynamic data uncertainties, such as standard uncertainty, combined standard uncertainty, combined expanded uncertainty, and different types of precision (e.g., repeatability, deviation from the fitted curve, or device specifications).

Establishment of the XML-based IUPAC standard will provide an easy-to-use and extremely efficient pipeline for transferring data from data producers to data users. The standard will serve as a hub tool and assure interoperability between various data management systems and operation platforms.

For more information, contact the Task Group Chairman Michael Frenkel <frenkel@boulder.nist.gov>.

www.iupac.org/projects/2002/2002-055-3-024.html

Chemical Thermodynamics for Industry

For over a century, chemical thermodynamics—the history of which stretches back 150 years—has been the foundation for much of chemistry. Despite this historical importance, there is an attitude among many chemists that thermodynamics has little relevance to modern day chemistry and will have little importance in the future development of chemistry. To counteract this view, the former IUPAC Commission on Chemical Thermodynamics, published in 1999 a volume entitled *Chemical Thermodynamics for the 21st Century*. It consisted of 27 chapters, all focusing on the applications of thermodynamics to very recent developments in chemistry. The aim was to highlight the role of thermodynamics at the forefront of chemical research.

In 2002, the International Association of Chemical Thermodynamics, the successor to the commission, decided to publish a collection of 25 essays on applied chemical thermodynamic topics. The aim of this publication is to highlight the role of thermodynamics in chemical industry and to show that it not only helps us understand the world we live in, but also

helps to create a better world. Among the topics to be covered in the new volume are the following:

- multiphase thermodynamics
- reactive distillation
- thermodynamic properties from *ab initio* quantum chemistry
- molecular modeling
- properties of clathrates
- ionic liquids in separation processes
- calorimetry
- transport properties
- bioseparation
- nano-particles and nano-technology

The volume will be published in 2004 with the Royal Society of Chemistry (UK). The editor is Professor Trevor Letcher, who edited the previous volume (*Chemical Thermodynamics for the 21st Century*, 1999 [ISBN 0-632-05127-2], <www.iupac.org/publications/books/author/letcher.html>). The new collection is aimed at those working in this field as well as general chemists, prospective researchers, and those involved in funding chemical research.

For more information, contact the Task Group Chairman Trevor Letcher <letcher@nu.ac.za>.

www.iupac.org/projects/2002/2002-063-1-100.html

Pesticide Science—Harmonization of Data Requirements and Evaluation

The IUPAC Chemistry and the Environment Division has had a sustained interest in pesticide science. The recent ***IUPAC-Korean Society of Pesticide Science International Workshop on Pesticides*** *was not only an integral project, but it was an occasion for reviewing other IUPAC projects in this field. In this article, Kenneth Racke reports on the workshop.*

More than 300 scientists, government regulators, and industry leaders representing 28 countries gathered in Seoul, Korea, 13–15 October 2003, to participate in the IUPAC-Korean Society of Pesticide Science International Workshop on Pesticides 2003.[1] The theme of the workshop was "Harmonization of Data Requirements and Evaluation."

The workshop was co-organized by the Korean Society of Pesticide Science (KSPS) and the IUPAC Division of Chemistry and the Environment (DCE). Cosponsors included the Korea Rural Development Administration, Korea Institute of Toxicology, Korea Crop Protection Association, CropLife Asia, and several additional national organizations. Dr. Byung-Youl Oh, president of KSPS, coordinated local arrangements. IUPAC contributions were coordinated by Dr. Yong-Hwa Kim of the DCE and myself.

Participants in the workshop had the opportunity to attend 33 invited lectures and view approximately 100 posters. Main program topics included "Pesticide Regulatory Harmonization," "Residue Behavior and Fate," and "Risk Assessment and Management." The program also included 12 IUPAC lecturers from the DCE Subcommittee on Crop Protection Chemistry, who highlighted the findings and recommendations of a number of recently concluded[2,3,4] and ongoing[5,6] IUPAC projects. Lectures were also presented by representatives of the Organisation for Economic Co-operation and Development (OECD), the Food and Agriculture Organization of the United Nations (FAO), the International Atomic Energy Agency, and Codex.

The workshop addressed pesticide residues on food.

Topics addressed at the workshop were diverse and included research reports on chemistry investigations, establishment of standards (food, water), toxicity characterization, risk assessment (dietary intake, occupational exposure, and ecological impacts), pesticide evaluation schemes, risk indicators and risk reduction, and standard formats for submissions and reviews. It was clear that there is a need to concentrate efforts and resources toward activities with the greatest benefit to all stakeholders. Participants also noted that perhaps the greatest challenges to be surmounted involve legislative and political barriers. A final workshop discussion session highlighted a series of overall observations and future considerations, and these are briefly summarized below.

First, the high-quality **research and monitoring** activities occurring within Korea and the surrounding countries were discussed at the workshop session.