Meeting Report

Interdivisional Discussion of the Critical Evaluation of Chemical Data

Organized as IUPAC Project 2016-043-1-500

11 July 2017
IUPAC General Assembly
Sao Paulo, Brazil

The following individuals participated in all or part of the meeting:

Ian Bruno, Subcommittee on Cheminformatics Data Standards, Committee on Publications and Cheminformatics Data Standards
Stuart Chalk, Subcommittee on Cheminformatics Data Standards, Committee on Publications and Cheminformatics Data Standards
Antony Davies, Subcommittee on Spectroscopy Data Standards, Committee on Publications and Cheminformatics Data Standards
Vladimir Gubala, Subcommittee on Toxicology and Risk Assessment, Division VII
Michael Hess, Subcommittee on Polymer Terminology, Division IV
Brynn Hibbert, Subcommittee on Solubility and Equilibrium Data, Division V
Robin Hutchinson, Subcommittee on Modeling of Polymerization Kinetics and Processes, Division IV
Clara Magalhaes, Subcommittee on Solubility and Equilibrium Data, Division V
David Martinsen, Subcommittee on Cheminformatics Data Standards, Committee on Publications and Cheminformatics Data Standards
Leah McEwen, Subcommittee on Cheminformatics Data Standards, Committee on Publications and Cheminformatics Data Standards
Greg Russell, Subcommittee on Modeling of Polymerization Kinetics and Processes, Division IV
David Shaw, Subcommittee on Solubility and Equilibrium Data, Division V
Earle Waghorne, Subcommittee on Solubility and Equilibrium Data, Division V
Thomas Walczyk, Subcommittee on Isotopic Abundance Measurements, Commission on Isotopic Abundances and Atomic Weights, Division II

Summaries of Current and Recent Activities in Critical Evaluation were presented by three groups within IUPAC active in data Evaluation

1. Critical Evaluation of Polymerization Kinetics Data (Subcommittee on Modeling of Polymerization Kinetics and Processes, Division IV)

   Robin Hutchinson gave a PowerPoint presentation of this project which has been running for three decades. His presentation is Attachment 1. Greg Russell also added a few comments.

2. Critical Evaluation of Isotopic Abundances and atomic weights (Commission on Isotopic Abundance Measurements and Atomic Weights, Division II)

   Thomas Walczyk discussed this work with emphasis on the metrological approach to measurement uncertainty as described in two documents, The Guide to the Expression of Uncertainty in Measurement (the GUM) and The International Vocabulary of Metrology (the VIM). Further information is available at <http://www.ciaaw.org>.

3. The Solubility Data Project (Subcommittee on Solubility and Equilibrium Data, Division V)

   David Shaw gave a summary of the Solubility Data Series (SDS), a collection of compilations and critical evaluations of solubilities in various systems. The SDS has been an ongoing project since the 1970s producing more than 100 volumes evaluating published data for chemically well defined systems of gases in liquids, liquids in liquids and solids in liquids. Further information is available at <https://iupac.org/who-we-are/divisions/division-details/?body_code=502>.

General Discussion

The bulk of the meeting was a wide ranging discussion of participants' experience, perspectives and challenges in critical evaluation. In this context several themes emerged. The goal of the meeting was to exchange ideas and perspectives; no attempt was made to reach consensus during the discussion. Consequently not all participants may agree with all thoughts expressed here.

- An essential goal of critical evaluation is to convey to data users, whatever their level of chemical sophistication, a well considered and supported estimate of the consensus value based on experimental results for the quantity under consideration

and of the level of uncertainty surrounding that value. The metrological approach to the expression of uncertainty is an important tool in this context.

- Advances in computer-based handling of scientific data are leading to new possibilities for data manipulation and interpretation. These advances also present new challenges of providing information about the data (meta-data) in formats that are assessable to both humans and computers.

- The delivery of data to users is presently in flux because of continuing rapid changes in electronic methods of data aggregation analysis and presentation. It is essential to make evaluated data available through channels that potential users prefer or at least will actually use.

- One topic not discussed during the meeting was whether meetings like this one should be repeated to encourage a continuing exchange of information and interdivisional projects. One form this could take would be an interdivisional working group or subcommittee on critical evaluation. The Task Group plans to discuss such possibilities with various interested parties and proceed as appropriate. Comments are welcome.

Note Added September 2017 by DGS:

Conversations during the SSED 2017 Annual Meeting and with participants in the Sao Paulo meeting by email indicates interest in the formation of Interdivisional Subcommittee on Critical Evaluation of Data with a first project of the preparation of a Technical Report describing best practices for critical evaluation of data.