

## Interdivisional Discussion of Critical Evaluation of Chemistry Data

The exhaustive compilation of the primary chemical literature of property data for systems and the critical evaluation of the resulting data sets by international teams of experts has long been a IUPAC activity. Thus, the current 'Guidelines for IUPAC Projects' states, "The core activity of IUPAC is to provide *critical evaluations of methods and data* and to make recommendations for nomenclature, terminology, metrology, and measurement standards" (*italics added*).

Prior to 2001, when IUPAC activities were organized around Commissions within the Divisions, a number of Commissions and of Subcommittees within Commissions focused on critical evaluation and constituted an ongoing pool of expertise in the critical evaluation of chemical data. According to the IUPAC Handbook 2000-2001, groups with ongoing interests in critical evaluation included the Subcommittee on Thermodynamic Data (within the Commission on Thermodynamics, I.2), the Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry (within the Commission on Chemical Kinetics, I.4), the Commission on Atomic Weights and Isotopic abundances (II.1), the Commission on Equilibrium Data (V.6), and the Commission on Solubility Data (V.8). Since the reorganization of IUPAC to a project-driven structure, three bodies have existed with a continuing focus on the compilation and critical evaluation of data—the Commission on Isotopic Abundances and Atomic Weights (II.1), the Subcommittee on Modeling of Polymerization Kinetics and Processes within the Polymer Division, and the Subcommittee on Solubility and Equilibrium Data (SSED) within the Analytical Chemistry Division. Additional critical evaluation of data is continuing in the Physical and Biophysical Chemistry Division without formal commission or subcommittee structure as a series of projects creating an evaluated database of kinetic data for atmospheric chemistry. Based on a review of the titles of active projects listed on the IUPAC web site in November 2016, it appears that one project involving critical evaluation of data is underway in the Physical and Biophysical Chemistry Division (Division I), three in the Inorganic Chemistry Division (Division II), five in the Polymer Division (Division IV), and 16 in the Analytical Chemistry Division (Division V).

Although data compilation and evaluation has continued in IUPAC to the present day, the breadth

of such work has diminished. The reason seems clear. In parts of IUPAC lacking individuals with experience and interest in data compilation and evaluation, the need for such projects may not be perceived or, when perceived, may be deemed too difficult to address. However, the full dimensions of this situation are unknown. Therefore, it seemed appropriate to bring together interested bodies and individuals to share information about plans and activities and to consider whether it would be useful to hold further meetings, possibly leading to a permanent structure that would share information and help focus attention.

The critical evaluation of data and the dissemination of data products to communicate evaluations to users is a complex undertaking. To better understand IUPAC's current activities and future opportunities in critical evaluation, the SSED organized an interdivisional discussion of the critical evaluation of chemical data as part of the General Assembly held in São Paulo, Brazil in July 2017. This open meeting attracted 14 participants from six Divisions and Committees to discuss ongoing activities and future needs in the area of critical evaluation. See IUPAC project 2016-043-1-500 for more details and for a meeting report.

The São Paulo meeting first heard descriptions of three current activities in critical evaluation. Robin Hutchinson spoke about the critical evaluation of polymerization kinetics data by the Subcommittee on Modeling of Polymerization Kinetics and Processes, Division IV. Thomas Walczyk discussed the critical evaluation of isotopic abundances and atomic weights by the Commission on Isotopic Abundance Measurements and Atomic Weights, Division II. David Shaw described critical evaluations prepared by the Solubility Data Project under the Subcommittee on Solubility and Equilibrium Data, Division V. Further information about these activities can be found in the meeting report.

Ian Bruno, Stuart Chalk, Tony Davies, and David Martinsen provided comments about the work of the Subcommittee on Cheminformatics Data Standards (SCDS) of the Committee on Publications and Cheminformatics Data Standards. For critically evaluated data to be incorporated more broadly into systems used by practicing chemists, they need to be digitally accessible, convenient for chemists, and processable by computer algorithms. SCDS is addressing organizational and technical infrastructure to support digital forms of IUPAC assets for improved access and use in the chemistry community, and is interested to collaborate with these division

projects on electronic delivery of critically evaluated data.

The bulk of the meeting was a wide-ranging discussion of participants' experiences, 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-supported estimate of the consensus value based on experimental results for the quantity under consideration and of the uncertainty associated with 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 enable more efficient handling and presentation of data and present new challenges in 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, as well as accessible for automated functions and collation.

Communication among meeting participants is continuing and interest is coalescing around two interdivisional activities. The first of these is assembling an interdivisional Task Group to prepare a Technical Report describing best practices for the critical evaluation of data. And the second is the establishment of an Interdivisional Subcommittee on Critical Evaluation of Data to continue the discussion of topics of mutual interest and to develop additional projects as the need arises. Wider participation in this interdivisional activity is welcome.

For further information, contact David Shaw <shaw02110@gmail.com>

[www.iupac.org/project/2016-043-1-500](http://www.iupac.org/project/2016-043-1-500)

## Middle east regional cooperation and sustainable water management of transboundary water

The Middle East is in turmoil in various ways, especially through the long-standing political crisis and conflicts affecting the people of the region. Widespread conflict and human rights violations, spurred by unsustainable water and energy

supplies, coupled with climate change, are causing the displacement of the population, as well as environmental migration. Poor conservation of the environment and inadequate treatment of pollutants led to the degradation of chronically depleted water resources and the trans-boundary movement of pollutants from one political entity to another, endangering the drinking water quality and contributing to the ongoing conflicts in the region. Thus, the role of water in improving human lives has never been more important, as stated by the UN Sustainable Development Goals (SDGs) [1]. The sustainable management of water resources and the quality of water in rivers, lakes, and aquifers plays a key role in meeting the challenge of climate change and in achieving a secure food supply and improved public health.

The continuous and severe drought over the past few years has raised water scarcity issues and water quality degradation in the region is worsening. As noted by Tal and Abed (2010) and by Schoenfeld (2011), the possibility of dealing with these issues requires experts detached from the political conflict and able to work across geopolitical borders. The involvement of scientists from neighboring nations and the international community is considered the right avenue to address regional issues [2,3].

**To review these issues**, a workshop titled, "Regional Cooperation and Sustainable Water Management of Transboundary Water", was organized with the support of IUPAC's Chemistry and the Environment Division. It took place in Malta, 10-15 December 2017, as part of the biennial Malta Conferences Foundation (MCF), MALTA VIII, "Frontiers of Science: Research and Education in the Middle East—a Bridge to Peace". This continues previous initiatives, including a prior program of workshops in collaboration with the MCF on regional water chemistry which yielded positive results and several publications and

