

Critical Evaluation of Homogeneous Equilibrium and Solubility Constants of Gadolinium in Environmental and Biological-Relevant Conditions

There are a number of trace elements that until recently were only considered to be laboratory curiosities but which have now become essential components in a variety of applications ranging from information and communication technologies, semiconductors, electronic displays and optic/photonic applications, and “green energy” related technologies. Their current strategic importance is such that these elements have now been labeled as “energy-critical elements” or “technology-critical elements” (TCEs) and initiatives at national levels are underway to secure their availability in the coming years. TCEs have diverse chemistries and uses. The degree of the current knowledge on their environmental fate and (eco)toxicity is not uniform, ranging from relatively well studied elements, such as the platinum group, to essentially unknown ones, such as tellurium. But for all of them, fundamental thermodynamic data are lacking.

This project will compile and critically evaluate existing data for gadolinium. This will allow a “best set” to be immediately used by stakeholders and sound identification of the systems that require urgent data acquisition. Gadolinium is an element of increasing concern because its concentration is steadily increasing in surface waters world-wide.

For more information and comments, contact Task Group Chair Montserrat Filella <montserrat.filella@unige.ch>.

<https://iupac.org/project/2018-025-1-500>

23rd UNESCO/IUPAC Postgraduate Course in Polymer Science

The UNESCO/IUPAC Postgraduate Course in Polymer Science has been organized annually since the academic year 1996–1997 by the Institute of Macromolecular Chemistry of the Czech Academy of Sciences (Prague, Czech Republic)—with financial support of the Czech Academy of Sciences and under the auspices of IUPAC and the Czech Commission for UNESCO.

The Institute has more than 60 years of experience in postgraduate polymer science education and offers up-to-date facilities for polymer science. The course lasts 10 months and comprises primarily experimental

work on research projects under supervision of institute scientists, compulsory lectures and laboratory demonstrations in modern polymer science, and access to all educational activities within the Institute. At the end of each run of the Course, all of the participants report on their project results in a public meeting, where a certificate bearing the logos of UNESCO and IUPAC is awarded to the participants—new graduates.

The Course is now a global activity with graduates from all continents except Australia and North America, represents a major educational activity within Polymer Division, and contributes to a positive image of IUPAC even outside the professional community. Reports on the courses have been presented annually and favorably accepted at the meetings of the IUPAC Polymer Division. The 22nd run (the year 2017–18) was completed by 10 participants at the end of July 2018. The 23rd Course started in October 2018 and covers the 2018–19 academic calendar. The Course was awarded the IUPAC-Samsung Education Prize for 2005, and received support from the Hanwha-Total fund once again this year.

For more information and comments, contact Task Group Chair Pavel Kratochvíl <krat@imc.cas.cz>

<https://iupac.org/project/2018-031-1-400>

Guidance for the Compilation, Critical Evaluation and Dissemination of Chemical Data

Critical evaluation of chemical data has long been an important activity within IUPAC. 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.” Members of the Analytical Chemistry Division’s Subcommittee on Solubility and Equilibrium Data, wanting to learn more about activities related to critical evaluation in other divisions and committees, organized an *ad hoc* interdivisional discussion on critical evaluation during the 2017 General Assembly (project 2016-043-1-500). This half-day meeting was attended by interested individuals from the Inorganic Chemistry Division (Div II), the Polymer Division (IV), the Analytical Chemistry Division (V), and the Committee on Publications and Cheminformatics Data Standards (CPCDS). From this meeting and subsequent conversations (which have included the Physical and Biophysical Chemistry Division (I)

and the Chemistry and the Environment Division (VI) as well as those listed above) two ideas emerged: that the exchange of information and experience among groups and individuals in IUPAC concerned with critical evaluation should continue, and that an important first project would be to develop guidance or best practices for critical evaluation of chemical data. This project addresses that second idea.

Currently active critical evaluation projects within IUPAC are highly varied treating both equilibrium and kinetic data; properties measured with either high and low relative uncertainty; and outputs ranging from monographs to databases. Given this range in the data sets evaluated and the rapidly evolving needs for cheminformatic documentation, guidance is needed to focus on best practices and provide flexibility while at the same time embodying high scientific standards.

The Task Group that has been assembled for this project reflects the breadth of IUPAC's experience in critical evaluation.

The Task Group will consider the three aspects of the critical evaluation process—compilation, evaluation, and dissemination—and develop best practice recommendations for each. Because of the wide variation in the data types that are evaluated, detailed protocols for the work are not considered appropriate. Rather the guidance will consider the qualities that are inherent in a good evaluation (completeness, clarity, traceability, *etc.*) and how those qualities can be achieved.

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<https://iupac.org/project/2018-009-2-500>



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