Making an imPACt

Recent IUPAC technical reports and recommendations that affect the many fields of pure and applied chemistry.
See also www.iupac.org/what-we-do/journals/

Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development (IUPAC Technical Report)

Paul Erhardt, Kenneth Bachmann, *et al.*
Pure and Applied Chemistry, 2021
Volume 93, Issue 3, pp. 273-403
https://doi.org/10.1515/pac-2018-0208

This project originated more than 15 years ago with the intent to produce a glossary of drug metabolism terms having definitions especially applicable for use by practicing medicinal chemists. A first-draft version underwent extensive beta-testing that, fortuitously, engaged international audiences in a wide range of disciplines involved in drug discovery and development. It became clear that the inclusion of information to enhance discussions among this mix of participants would be even more valuable. The present version retains a chemical structure theme while expanding tutorial comments that aim to bridge the various perspectives that may arise during interdisciplinary communications about a given term. This glossary is intended to be educational for early stage researchers, as well as useful for investigators at various levels who participate on today's highly multidisciplinary, collaborative small molecule drug discovery teams.

https://iupac.org/project/2000-009-1-700

Interpretation and use of standard atomic weights (IUPAC Technical Report)

Adriann M.H. van der Veen, Juris Meija, Antonio Possolo, and David Brynn Hibbert
Pure and Applied Chemistry, 2021
Volume 93, Issue 5, pp. 629-646
https://doi.org/10.1515/pac-2017-1002

Many calculations for science or trade require the evaluation and propagation of measurement uncertainty. Although relative atomic masses (standard atomic weights) of elements in normal terrestrial materials and chemicals are widely used in science, the uncertainties associated with these values are not well understood. In this technical report, guidelines for the use of standard atomic weights are given. This use involves the derivation of a value and a standard uncertainty from a standard atomic weight, which is explained in accordance with the requirements of the Guide to the Expression of Uncertainty in Measurement. Both the use of standard atomic weights with the law of propagation of uncertainty and the Monte Carlo method are described. Furthermore, methods are provided for calculating uncertainties of relative molecular masses of substances and their mixtures. Methods are also outlined to compute material-specific atomic weights whose associated uncertainty may be smaller than the uncertainty associated with the standard atomic weights.

https://iupac.org/project/2013-032-1-200

Glossary of methods and terms used in analytical spectroscopy (IUPAC Recommendations 2019)

Heidi Goenaga Infante, John Warren, *et al.*
Pure and Applied Chemistry, 2021
Volume 93, Issue 6, pp. 647-776
https://doi.org/10.1515/pac-2019-0203

Recommendations are given concerning the terminology of concepts and methods used in spectroscopy in analytical chemistry, covering nuclear magnetic resonance spectroscopy, atomic spectroscopy, and vibrational spectroscopy.

https://iupac.org/project/2017-027-1-500

The Gender Gap in Science: PAC Special Topics Issue

Mark Cesa and Mei-Hung Chiu, co-editors
Pure and Applied Chemistry, 2021
Volume 93, Issue 8, pp. 829-961

In a recent article in *Chemistry International* (Chiu and Cesa, *Chem. Int.* 2020, 42(3), 16-21; https://doi.org/10.1515/ci-2020-0306) we reported on the results of the Gender Gap Project. The project, entitled, "A Global Approach to the Gender Gap in Mathematical, Computing, and Natural Sciences: How to Measure It, How to Reduce It?" (https://gender-gap-in-science.org/), was funded by the International Science Council (ISC, formerly ICSU) and was co-led by IUPAC and the International Mathematical Union, IMU. The results of the project clearly showed that women continue to have less positive experiences than men in education and employment across scientific disciplines, geographic regions, and levels of economic development

(https://gender-gap-in-science.org/2020/06/25/gender-gap-in-science-book/). At the final project conference at the International Center for Theoretical Physics, ICTP, in Trieste, Italy, a series of recommendations for improving gender awareness for scientific unions, local organizations, and instructors and parents was prepared and disseminated (https://gender-gap-in-science.org/project-book-booklet/).

The project partners and participants at the final conference contributed a range of approaches to reducing the gender gap in science and improving gender equity in their fields. To raise awareness among chemists about these perspectives, we invited sixteen persons from a range of scientific, mathematical and computing disciplines to prepare articles for a special topics issue of *Pure and Applied Chemistry*. This issue explores the results of the Global Survey; describes initiatives to reduce the gender gap in astronomy, biology, chemistry, computing machinery, mathematics, ocean science, and physics; includes regional approaches to reducing the gender gap, particularly in the developing world; and proposes new and innovative approaches that include networking initiatives and collections of good practices around the world for encouraging girls and young women to pursue careers in science.

Work in IUPAC on the reducing the gender gap in science continues. In 2020 the Standing Committee for Gender Equality in Science, SCGES (https://gender-equality-in-science.org/), was instituted, with IUPAC is a founding member along with fifteen other international partners. A current IUPAC project (https://iupac.org/project/2020-016-3-020) includes analysis of the Gender Gap project survey data specific to the chemical science, a compilation of good practices in reducing the gender gap, and participating in an initiative by several scientific publishers to examine gender trends.

Reference materials for phase equilibrium studies. 1. Liquid–liquid equilibria (IUPAC Technical Report)

Ala Bazyleva, William E. Acree, *et al.*
Pure and Applied Chemistry, 2021
Volume 93, Issue 7, pp. 811-827
https://doi.org/10.1515/pac-2020-0905

This article is the first of three projected IUPAC Technical Reports resulting from IUPAC Project 2011-037-2-100 (Reference Materials for Phase Equilibrium Studies). The goal of this project is to select reference systems with critically evaluated property values for the validation of instruments and techniques used in phase equilibrium studies of mixtures. This report proposes seven systems for liquid–liquid equilibrium studies, covering the four most common categories of binary mixtures: aqueous systems of moderate solubility, non-aqueous systems, systems with low solubility, and systems with ionic liquids. For each system, the available literature sources, accepted data, smoothing equations, and estimated uncertainties are given.

https://iupac.org/project/2011-037-2-100

Special CTI on Polymer Sciences

A special issue of *Chemistry Teacher International* has been released, resulting of a collaboration project between the Sub-committee on Polymer Education part of the IUPAC Polymer Division, and the IUPAC Committee on Chemistry Education.

CTI, Volume 3, Issue 2
June 30, 2021; https://www.degruyter.com/journal/key/CTI/3/2/html

This special issue, co-edited by Chin Han Chan and Jan Apotheker, contains articles which are intended to bridge the gap between research and education. The idea is to share the good practices for some topics in polymer sciences for educational purposes. We hope that lecturers at the universities may refer to these articles as the references to teach or lecture young researchers. Another purpose is to inform the high-school/pre-university teachers about recent developments in polymer chemistry, so that they may introduce some of the topics in this issue to students.

The articles are based on the lecture notes presented at IUPAC Education Workshops in Polymer Sciences (2016, 2017, 2018, and 2020+) and educational materials in polymer sciences covering topics of polymer synthesis (three articles), polymer characterization (five articles), polymer processing (two articles) and polymer applications and others (three articles). The educational materials shared in this special issue have been previously used by researchers with the aim of promoting polymer sciences.

Issue preface published Online April 2; 2021 https://doi.org/10.1515/cti-2021-0008