Definitions and preferred symbols for mass diffusion coefficients in multi-component fluid mixtures including electrolytes (IUPAC Technical Report)

Tobias Klein, Chathura J. Kankanamge, Thomas M. Koller, Michael H. Rausch, Andreas P. Fröba, Marc J. Assael, William A. Wakeham, Gabriela Guevara-Carrion and Jadran Vrabec

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This work summarizes the fundamentals of the description of molecular diffusion in liquid and gaseous non-electrolyte and electrolyte systems at constant temperature and pressure and in the absence of external fields. On the basis of Fick's law and the theory of Maxwell and Stefan, the description of diffusive fluxes in commonly used reference frames and a recommendation for the terminology of the associated diffusion coefficients are given. For non-electrolyte systems, the corresponding equations for the diffusive fluxes are outlined for a general *n*-component mixture and are explicitly stated for binary and ternary mixtures. Additionally, the transformation of the component order is discussed for a general *n*-component mixture. For electrolyte mixtures, explicit equations for the diffusive fluxes are stated for binary mixtures consisting of a molecular solvent and a dissolved electrolyte component and binary mixtures consisting of two electrolyte components sharing a common ion. Furthermore, explicit equations for the diffusive fluxes are given for ternary systems consisting of one electrolyte component dissolved in two non-electrolyte solvents. For all the aforementioned systems, transformations of the diffusion coefficients between commonly used reference frames are included.

https://iupac.org/project/2014-010-1-100/

IUPAC/CITAC guide: interlaboratory comparison of categorical characteristics of a substance, material, or object (IUPAC Technical Report)

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This Guide is intended for harmonization of interlaboratory comparisons of categorical— nominal (qualitative, *i.e.,* non-quantitative) and ordinal (semi-quantitative)— characteristics of a substance, material, or object. It provides guidance for application of relevant methods of mathematical statistics for design of such interlaboratory comparisons and analysis of the obtained data, when the methods developed for continuous quantitative values (*e.g.,* ANOVA—analysis of variance) cannot be used without violation of their basic assumptions. The proposed approach employs recently-developed two-way nominal analysis of variation CATANOVA and two-way ordinal analysis of variation ORDANOVA. The Guide also addresses correlation between the categorical characteristics, as well as correlation between these characteristics and the chemical composition of the material or object. A multisensory quality index of a product, combining information on its categorical characteristics, is detailed. It allows for comparison of the quality of the same material produced by different producers. The examples provided in the Guide are from the fields of macroscopic examination of weld imperfections, comparison of odor intensity of drinking water, and comparison of sensory (ordinal) characteristics of a sausage. A corresponding calculation tool with an Excel spreadsheet including macros, and programs written in the R environment, are available in the specified references.

https://iupac.org/project/2021-017-2-500/
https://iupac.org/project/2023-016-1-500/

Blockchain technology: driving change in the scientific research workflow

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The goal of this white paper is to present an objective overview of the current use of blockchain technology along the scientific research workflow and in related areas such as chemical/drug supply chains and education. It represents the culmination of three years of data gathering, including input from multiple interviews with pioneer users of the technology, as well as from more recent adopters around the globe, and recent industry technology analysts' reports. Within these

pages are descriptions of successful applications of the technology at each step of the scientific research workflow—from the timestamping of ideas to funding, to actual experimentation, to the analysis of research results, and ultimately to the sharing of information and the publication of results. However, not all blockchain use cases have such a successful conclusion. In this white paper you will learn where the technology has not worked—and why—thanks to those interviewed who discussed in detail the lessons that they themselves learned during their own blockchain journey. In addition, the paper highlights the potential future uses of the technology; the pitfalls to avoid when considering its use; when and how legislation and regulatory policies come into play; and how the technology is evolving and growing stronger (some say that the fourth generation of the blockchain evolution is on the horizon!). The paper also discusses parallel developments in quantum computing, its potential impact on blockchain technology, and what developments are in progress to ensure a stable and provably secure, quantum safe alternative to the existing blockchain approaches.

https://iupac.org/project/2023-009-1-024/

Let's celebrate IYQ

The 2025 International Year of Quantum Science and Technology (IYQ) recognizes 100 years since the initial development of quantum mechanics <quantum2025.org>. Joining in the celebrations, IUPAC has prepared a special Issue of *Pure and Applied Chemistry*, containing about 40 invited articles that recognize the impact of quantum science and technology in many branches of chemistry. The Guest Editors are Manuel Yáñez (manuel.yanez@uam.es), Autonomous University of Madrid, Spain and Russell J. Boyd (russell.boyd@dal.ca), Dalhousie University, Canada.

INTERNATIONAL YEAR OF
Quantum Science and Technology

IUPAC Provisional Recommendations

Provisional Recommendations are preliminary drafts of IUPAC recommendations. These drafts encompass topics including terminology, nomenclature, and symbols. Following approval, the final recommendations are published in IUPAC's journal *Pure and Applied Chemistry* (PAC) or in IUPAC books. During the commentary period for Provisional Recommendations, interested parties are encouraged to suggest revisions to the recommendation's author. https://iupac.org/recommendations/under-review-by-the-public/

Basic Classification and Definitions of Polymerization Reactions

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This document provides recommendations addressing the long-standing dilemma of the wide variety of terms that are used to describe the two common classes of polymerization mechanisms in the scientific literature, which includes chemistry and polymer-science textbooks. It is an update of a 1994 IUPAC document on this topic and provides clarification and hierarchical structure regarding the basic classification and terminology describing polymerization reactions. The term step polymerization describes polymerizations in which growth occurs by reactions between monomer, oligomer, or polymer molecules of any length. We clearly denote here the two subclasses of step polymerization: additive step polymerization (synonym: polyaddition) and condensative step polymerization (synonym: polycondensation). The term chain polymerization describes polymerizations that proceed via a chain reaction with monomer molecules adding to active sites on polymer chains. Subclasses of chain polymerization include additive chain polymerization and condensative chain polymerization. The terms provide a logical and straightforward structure for describing the two common classes of polymerization mechanisms. Previously defined terms relevant to these two classes of polymerization reactions are also replicated in this Recommendation document.

Comments by 30 November 2025

https://iupac.org/recommendation/basic-classification-and-definitions-of-polymerization-reactions/