Terms of Latin origin relating to sample characterization (IUPAC Technical Report)

Vanessa K. Peterson, Matteo Bianchini, Karena W. Chapman, Martina Elice, David Brynn Hibbert, Paul Roche, Luigi Silvano, Lorenzo Stievano
Pure and Applied Chemistry, 2024
Vol. 96, no. 11, 2024, pp. 1531-1540
https://doi.org/10.1515/pac-2022-1103

The use of Latin origin terms, relevant for sample characterization modalities, is described with a focus on samples under controlled conditions, samples within devices, and samples during physico-chemical evolution. The terms *in vitro*, *in vivo*, *in situ*, *ab initio*, *in silico*, *post mortem*, *ex situ*, *posthumous*, *in vacuo*, *(in) operando*, *post facto*, and *ex post facto*, as used in the scientific literature, are considered. Uses of the Latin origin terms *in situ*, *extra situm*, *in operando*, *in vivo*, *in vacuo*, *in vitro*, *extra vivum*, *post facto* and *ex post facto*, *ab initiis*, *computatro*, and *post mortem* are discussed. It is suggested that these terms are to be used without hyphenation and that all Latin derived terms are set in italic font.

https://iupac.org/project/2021-009-2-500/

Glossary of terms used in biochar research (IUPAC Technical Report)

Fotis Bilias, Divine Damertey Sewu, Seung Han Woo, Ioannis Anastopoulos, Frank Verheijen, Johannes Lehmann, Wenceslau Geraldes Teixeira, Dionisios Gasparatos, Kathleen Draper and Dimitrios Kalderis
Pure and Applied Chemistry, 2014
Vol. 96, no. 11, 2024, pp. 1541-1572
https://doi.org/10.1515/pac-2021-0106

Biochar is the solid carbonaceous product of biomass pyrolysis. The properties of biochar depend on the biomass feedstock as well as the pyrolysis temperature and time. Therefore, biochars with different properties and functionalities can be produced. Biochar research has been intensive in the past 15 years, focusing mainly on soil applications, wastewater treatment, and contaminant remediation. However, a formal definition of biochar and related terms is missing, which hinders the standardization of scientific results worldwide and the scaling-up of research at the industrial level. Furthermore, an official terminology may promote the development of a harmonized legal framework for biochar production and applications, both at regional and national levels. This glossary of terms consists of 178 scientifically sound definitions of the most commonly used terms in biochar research. The definitions of this glossary are interconnected, allowing the reader to further explore the synergies between terms. The distribution of terms reflects the multidisciplinarity of biochar research: chemistry, material science and engineering, and soil science are the main disciplines represented here. The list of terms is by no means exhaustive and the strategic objective of this effort is to develop a dynamic document in which more terms will be added in the future, and the existing ones will be refined, as biochar research evolves.

https://iupac.org/project/2015-056-3-600/

Properties and units in the clinical laboratory sciences. Part XXVIII. NPU codes for characterizing subpopulations of the hematopoietic lineage, described from their clusters of differentiation molecules (IUPAC Technical Report)

Evita Maria Lindholm, Eli Taraldsrud, Jakob Thaning Bay, Mats Bemark, Jens Magnus Bernth Jensen, Rebecca Ceder, Elisabeth Abrahamsen, Fatma Meric Yilmaz, Sridevi Devaraj, Eline van der Hagen and Helle Møller Johannessen
Pure and Applied Chemistry, 2024
Vol. 96, no. 11, 2024, pp. 1573-1582
https://doi.org/10.1515/pac-2023-0806

Examination results from clinical laboratories in the health area has increased through the last decades. Coding of laboratory analyses is an efficient way of securing standardized and accurate recording of patient information, which can then serve as an invaluable resource for clinical treatment decisions, improved patient care and medical research. The Nomenclature for Properties and Units (NPU) terminology was developed to support correct and standardized exchange of data across laboratories and ehealth systems. Use of the NPU terminology allows clinical examination results to be recognized, compared, reused in calculations, extracted for research or statistics, and stored for documentation, without loss of meaning. The terminology has been developed since the 1990's with support from the international organizations IFCC (International

Federation of Clinical Chemistry and Laboratory Medicine) in collaboration with IUPAC (International Union of Pure and Applied Chemistry).

Numerous diseases are associated with alterations in peripheral blood lymphocyte subpopulations, and the need to communicate the different cell types and differentiation states is therefore of outmost importance for clinical decisions in diagnosis, prognosis, and patient monitoring. Hematopoietic stem cells (HSCs) are multipotent, self-renewing progenitor cells from which all differentiated blood cell types arise during the process of hematopoiesis. These cells include lymphocytes, granulocytes, and macrophages of the immune system, as well as circulating erythrocytes and platelets. The lymphocytes, with the two distinct classes of B- and T-cells, constitutes the core of the adaptive immune system. And the differentiation of T-cells into effector and memory subsets represents a fundamental role in our ability to fight viruses or tumors, and our capacity to expand rapidly upon a secondary stimulation.

This document describes how the Nomenclature for Properties and Units (NPU) terminology can be applied to differentiate between cell subpopulations of the hematopoietic lineage. The clusters of differentiation molecules are included in the NPU syntax, together with its correct affiliations to indicate their presence or absence. This allows for identification and isolation of cell populations, subsets, and differentiation stages, which is essential for correct diagnosis and treatment of several malignancies and autoimmune diseases.

https://iupac.org/project/2021-022-1-700/

Definition of materials chemistry (IUPAC Recommendations 2024)

Milan Drábik, Robin T. Macaluso, Lukáš Krivosudský and Lidia Armelao
Pure and Applied Chemistry, 2024
Vol. 96, no. 12, 2024, pp. 1693-1698
https://doi.org/10.1515/pac-2023-0215

Materials chemistry is focused on the design, preparation, and understanding of innovative materials. It is an emerging area of research where definitions are not well established. This document defines the area of materials chemistry for the benefit of chemistry communities and the general public worldwide interested in this discipline. This recommendation defines the term "materials chemistry" as the "scientific discipline that designs, synthesizes, and characterizes materials, with particular interest on processing and understanding of useful or potentially useful properties displayed by the materials designed and synthesized for specific applications."

https://iupac.org/project/2020-022-1-200/

IUPAC Recommendations: (Un)equivocal Understanding of Hydrogen and Halogen Bonds and Their (Un)equivocal Naming!

Elangannan Arunan, Pierangelo Metrangolo, Giuseppe Resnati, and Steve Scheiner
Cryst. Growth Des. 2024, 24, 20, 8153–8158
https://doi.org/10.1021/acs.cgd.4c00982

This manuscript shows that Si-H hydrogen acts as a donor of electron density to halogen atoms in Me_3Si-H···Y complexes (Y = CF_3I, BrCN), thus proving that, consistent with IUPAC definitions of hydrogen and halogen bonds, hydridic hydrogen functions as a halogen bond acceptor. This has been necessitated by a paper recently published asking whether the definition of hydrogen bonding should be revised to include hydridic H atoms acting as electron donors. The authors discuss the various nomenclatures used for referring to intermolecular/noncovalent bonds formed by various elements and point out the convention established in naming them by IUPAC, after long deliberations among the chemists from all over the world.

IUPAC has so far approved the definitions of hydrogen bond (https://doi.org/10.1351/PAC-REC-10-01-02), halogen bond (Group 17; https://doi.org/10.1351/PAC-REC-12-05-10), chalcogen bond (Group 16; https://doi.org/10.1515/pac-2018-0713), and pnictogen bond (Group 15; https://doi.org/10.1515/pac-2020-1002). As one can see, except for hydrogen bond, other names indicate a group of elements. Any proposed new name underwent a very rigorous process with multiple rounds of peer-review and involved the whole chemistry community being open for public comment before acceptance.

https://iupac.org/project/2016-001-2-300/ and former projects referred therein.