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Steel and steel products — Vocabulary relating to chemical analysis

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Foreword

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This document was prepared by Technical Committee ISO/TC 17, *Steel*, Subcommittee SC 1, *Methods of determination of chemical composition*.

Any feedback or questions on this document should be directed to the user’s national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

To ensure that communication in a particular domain is effective and that difficulties in understanding are minimized, it is essential that the various participants use the same concepts and concept representations. Unambiguous communication related to analytical chemistry concepts is crucial given the implications that can arise from misunderstandings with regard to equipment.

Different levels of scientific and technical knowledge can lead to widely divergent understandings and assumptions about concepts. The result is poor communication that can lead into an increase of the risk of accidents and duplication of efforts as different define concepts according to their perspectives.

Conceptual arrangement of terms and definitions is based on concepts systems that show corresponding relationships analytical chemistry concepts. Such arrangement provides users with a structured view of the analytical methods and will facilitate common understanding of all related concepts. Besides, concepts systems and conceptual arrangement of terminological data will be helpful to any kind of user because it will promote clear, accurate and useful communication.

Steel and steel products — Vocabulary relating to chemical analysis

1 Scope

This document defines terms relating to methods of the determination of the chemical composition of steel and steel products.

2 Normative references

There are no normative references in this document.

3 Terms and definitions

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at https://www.iso.org/obp
- IEC Electropedia: available at https://www.electropedia.org/

3.1 General terms related to steel and cast iron

3.1.1
alloy steel
steel (3.1.17), other than a stainless steel, that conforms to a specification that requires one or more of the following elements, by mass percent, to have a minimum content equal to or greater than: 0,30 for aluminum; 0,000 8 for boron; 0,30 for chromium; 0,30 for cobalt; 0,40 for copper; 0,40 for lead; 1,65 for manganese; 0,08 for molybdenum; 0,30 for nickel; 0,06 for niobium (columbium); 0,60 for silicon; 0,05 for titanium; 0,30 for tungsten (wolfram); 0,10 for vanadium; 0,05 for zirconium; or 0,10 for any other alloying element, except sulphur, phosphorus, carbon, and nitrogen

[SOURCE: ASTM A941:2018]

3.1.2
austenitic steel
steel (3.1.17) where the structure consists of *austenite* (3.1.3) at ambient temperature

Note 1 to entry: Cast austenitic steels can contain up to about 20 % of *ferrite* (3.1.8).

3.1.3
austenite
solid solution of one or more elements in gamma iron (3.1.19)

3.1.4
boriding
thermochemical treatment of a workpiece to enrich the surface of a workpiece with boron

Note 1 to entry: The medium in which boriding takes place should be specified, e.g. pack boriding, paste boriding, etc.

3.1.5
cast/heat analysis

chemical analysis determined by the steel producer as being representative of a specific heat of *steel* (3.1.17)

Note 1 to entry: Where the analysis reported by the steel producer is not sufficiently complete for conformance with the *heat analysis* (3.1.5) requirements of the applicable product specification to be fully assessed, the manufacturer can complete the assessment of conformance with such *heat analysis* (3.1.5) requirements by using a *product analysis* (3.1.16) for the specified elements that were not reported by the steel producer, provided that *product analysis* (3.1.16) tolerances are not applied and the *heat analysis* (3.1.5) is not altered

[SOURCE: ASTM A941:2018]

3.1.6
cast iron

alloy of iron, carbon and silicon where the carbon content is approximately more than 2 %

3.1.7
ductile iron

nodular cast iron

cast iron (3.1.6) that has been treated while molten with an element (usually magnesium or cerium) that spheroidizes the graphite

[SOURCE: ISO 15156-2:2020, 3.5.4]

3.1.8
ferrite

body-centred cubic lattice structure of iron or *steel* (3.1.17)

3.1.9
forged steel

steel (3.1.17) product obtained by forging and that does not undergo subsequent hot conversion

Note 1 to entry: These products are mainly in the form of circles or squares.

3.1.10
grey cast iron

cast material, mainly iron and carbon based, carbon being present mainly in the form of flake (lamellar) graphite particles

Note 1 to entry: Grey cast iron is also known as flake graphite cast iron, and less commonly as lamellar graphite cast iron.

Note 2 to entry: Graphite form, distribution and size are specified in ISO 945-1.

[SOURCE: EN 1561:2011, 3.1]

3.1.11
killed steel

steel (3.1.17) deoxidized to such a level that essentially no reaction occurred between carbon and oxygen during solidification

[SOURCE: ASTM A941:2018]

3.1.12
malleable iron

white cast iron (3.1.18) that is thermally treated to convert most or all of the cementite to graphite (temper carbon)

[SOURCE: ISO 15156-2:2020, 3.5.3]

3.1.13
martensite
(phase) formed in carbon containing *steels* (3.1.17) by the cooling of *austenite* (3.1.3) at such a high rate that carbon atoms do not have time to diffuse out of the crystal structure in large enough quantities to form cementite (Fe_3C)

3.1.14
nitriding
case-hardening process in which nitrogen is introduced into the surface of metallic materials (most commonly ferrous alloys)

EXAMPLE Liquid nitriding, gas nitriding, ion nitriding and *plasma* (3.6.32) nitriding.

[SOURCE: ISO 15156-2:2020, 3.11]

3.1.15
non-alloyed steel
steel in which the percentage of each element is less than specific limiting values specified

Note 1 to entry: See Table in ISO 4948-1:1982, 3.1.2.

3.1.16
product analysis
chemical analysis carried out on a sample of the product taken after the final hot rolling operation

3.1.17
steel
ferrous material the principal element of which is iron and the carbon content of which is not more than 2 % of mass

Note 1 to entry: The presence of large quantities of carbide-forming elements can modify the upper limit of the carbon content.

Note 2 to entry: The nomenclature for unalloyed steels suitable for heat treatment and for alloyed steels is given in ISO 4948-1 and ISO 4948-2.

Note 3 to entry: Small amount of alloying elements added to non-alloy steels can cause the product to be defined as a micro-alloy steel.

3.1.18
white cast iron
cast iron (3.1.6) that displays a white fracture surface due to the presence of cementite

[SOURCE: ISO 15156-2:2020, 3.5.2]

3.1.19
gamma iron
pure iron with face-centred cubic lattice structure

3.2 General terms related to preparation of steel and cast iron

3.2.1
grinding
method of preparing a sample of metal for a physical method of analysis in which the surface of the *test sample* (3.3.15) is abraded using an abrasive wheel

3.2.2
linishing
method of preparing a sample of metal for a physical method of analysis in which the surface of the *test sample* (3.3.15) is abraded using a flexible rotating disc or continuous belt coated with an abrasive substance

3.2.3

milling

method of preparing sample chips or the surface of a sample for a physical method of analysis in which the surface of the sample is machined using a rotating, multi-edged cutting tool

3.3 General terms related to sample and sampling

3.3.1

aliquot

known amount of a homogeneous material, assumed to be taken with negligible sampling error

Note 1 to entry: The term "aliquot" is usually applied to fluids.

Note 2 to entry: The term "aliquot" is usually used when the fractional part is an exact divisor of the whole; the term "aliquant" has been used when the fractional part is not exact divisor of the whole (e.g. a 15 ml portion is an aliquant of 100 ml).

Note 3 to entry: When a *laboratory sample* (3.3.7) or a *test sample* (3.3.15) is "aliquoted" or otherwise subdivided, the portions have been called split samples.

3.3.2

analyte

component of a system to be analysed

[SOURCE: PAC, 1989, 61, 1657 (Nomenclature for automated and mechanised analysis (Recommendations 1989))]

3.3.3

analytical sample

sample prepared from the *laboratory sample* (3.3.7) and from which analytical portions can be taken

Note 1 to entry: The analytical sample can be subjected to various treatments before an analytical portion is taken.

Note 2 to entry: Where no homogenization or subdivision is necessary, the *laboratory sample* (3.3.7), the *test sample* (3.3.15), and, if the latter requires no further chemical or physical treatment, the analytical samples are identical. With some homogeneous materials such as waters or oils, the *laboratory sample* (3.3.7) may be taken directly from a sample unit and, if no further subdivision or homogenization is carried out, the *laboratory sample* (3.3.7) is the *test sample* (3.3.15). Similarly, with atmospheric particulates collected on a filter, the sample unit is the *laboratory sample* (3.3.7) and, if no further subdivision or homogenization is carried out, also the *test sample* (3.3.15).

[SOURCE: ISO 15193:2009, 3.3, modified — Note to entry added.]

3.3.4

consignment

quantity of metal delivered at one time

3.3.5

duplicate samples

replicate samples

multiple (or two) samples taken under comparable conditions

Note 1 to entry: This selection can be accomplished by taking units adjacent in time or space. Although the replicate samples are expected to be identical, often the only thing replicated is the act of taking the physical sample. A duplicate sample is a replicate sample consisting of two portions. The umpire samples usually used to settle a dispute; the replicate sample is usually used to estimate sample variability.

[SOURCE: PAC, 1990, 62, 1193 (Nomenclature for sampling in analytical chemistry (Recommendations 1990))]

3.3.6
increment

quantity of metal obtained by sampling at one time from a *consignment* (3.3.4)

3.3.7
laboratory sample

sample or *subsample(s)* (3.3.13) sent to or received by the laboratory

Note 1 to entry: When the laboratory sample is further prepared (reduced) by subdividing, mixing, *grinding* (3.2.1), or by combinations of these operations, the result is the *test sample* (3.3.15). When no preparation of the laboratory sample is required, the laboratory sample is the *test sample* (3.3.15). A *test portion* (3.3.14) is removed from the *test sample* (3.3.15) for the performance of the test or for analysis.

Note 2 to entry: The laboratory sample is the final sample from the point of view of sample collection but it is the initial sample from the point of view of the laboratory.

Note 3 to entry: Several laboratory samples can be prepared and sent to different laboratories or to the same laboratory for different purposes. When sent to the same laboratory, the set is generally considered as a single laboratory sample and is documented as a single sample.

[SOURCE: IUPAC orange book: 2002, 18.3.6, Sampling stages]

3.3.8
lot

quantity of material that is assumed to be a single population for sampling purposes

[SOURCE: PAC, 1990, 62, 1193 (Nomenclature for sampling in analytical chemistry (Recommendations 1990))]

3.3.9
matrix

components of the sample other than the *analyte* (3.3.2)

Note 1 to entry: to entry. In analysis.

[SOURCE: PAC, 1989, 61, 1657 (Nomenclature for automated and mechanised analysis (Recommendations 1989))]

3.3.10
primary sample

collection of one or more *increments* (3.3.6) or units initially taken from a population

Note 1 to entry: The portions can be either combined (composited or bulked sample) or kept separate (gross sample). If combined and mixed to homogeneity, it is a blended bulk sample.

Note 2 to entry: The term "bulk sample" is commonly used in the sampling literature as the sample formed by combining *increments* (3.3.6). The term "bulk sample" is ambiguous since it could also mean a sample from a bulk *lot* (3.3.8) and it does not indicate whether the *increments* (3.3.6) or units are kept separate or combined. Such use should be discouraged because less ambiguous alternative expressions (composite sample, aggregate sample) are available.

Note 3 to entry: "Lot sample" and "batch sample" have also been used for this concept, but they are self-limiting terms.

Note 4 to entry: The use of "primary" in this sense is not meant to imply the necessity for multistage sampling.

[SOURCE: IUPAC orange book: 2002, 18.3.6, Sampling stages]

3.3.11
representative sample

sample that has the same properties as a defined batch of material and represents the bulk material, within a defined confidence limit

[SOURCE: ISO 14488:2007, 3.7]

3.3.12
specimen
one or more pieces taken from each product in the sample, for the purpose of producing test pieces

[SOURCE: ISO 6361-1:2011, 3.7]

3.3.13
subsample
sample obtained by procedures in which the items of interest are randomly distributed in parts of equal or unequal size

Note 1 to entry: A sub-sample can be any of the following:

a) a portion of the sample obtained by selection or division;

b) an individual unit of the *lot* (3.3.8) taken as part of the sample;

c) the final unit of multistage sampling.

Note 2 to entry: The term “subsample” is used either in the sense of a “sample of a sample” or as a synonym for “unit”. In practice, the meaning is usually apparent from the context or is defined.

[SOURCE: ISO 11074:2015, 4.1.34]

3.3.14
test portion
part of the test sample, or part of the sample taken from the melt, submitted to analysis, in certain cases, the test portion can be selected from the sample product itself

Note 1 to entry: The following special types of test portions in the form of a solid mass obtained from a probe sample are distinguished

- disc originating from the sampling of molten metal (from a special sampler or a small ingot), used for OES or XRF
- test portion in the shape of a small disc, commonly described as a slug, obtained by punching,
- test portion in the form of a small appendage, commonly described as a lug,
- test portion in the form of a small-diameter rod, commonly described as a pin, obtained by cutting.

Note 2 to entry: When the test sample is in the form of chips or powder, or when a sample in the form of a solid mass is analysed by a thermal method, the *test portion* (3.3.14) is obtained by weighing. In the case of a physical method of analysis, the part actually analysed will constitute only a small mass of the test sample. In an optical emission spectrometric method, the mass of metal consumed in an electrical *discharge* (3.6.14) is about 0,5 mg to 1 mg, in an X-ray fluorescence spectrometric method, the characteristic radiation is produced from a very thin surface layer of the sample.

3.3.15
test sample
sample taken or formed from the *laboratory sample* (3.3.7), by a process involving homogenization using physical or mechanical treatments such as *grinding* (3.2.1), drilling, *milling* (3.2.3) or sieving

Note 1 to entry: The test sample is then in a form suitable for subsampling for analytical purposes, for storing for future analysis or for using for test purposes other than analytical.

[SOURCE: IUPAC orange book: 2002, 10.3.4.9]

3.3.16
test solution
analytical solution
solution prepared by dissolving, with or without reaction, the *test portion* (3.3.14) in a liquid

[SOURCE: IUPAC orange book: 2002, 18.3.6 Sampling stages]

3.3.17

trace element

element having an average concentration of less than about 100 parts per million atoms (ppm) or less than 0,01 % by weight

[SOURCE: PAC, 1979, 51, 2243 (General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)]

3.4 General terms related to analytical standards

3.4.1

blank test solution

solution that contains all the chemicals except for the element to be determined in the same concentration as required for the preparation of a *reference standard solution* (3.4.17) of that element

[SOURCE: OIML R 100-1:2013, 3.3.2]

3.4.2

blank reference solution

solution used to set the zero absorbance on the *spectrometer* (3.5.22) and that normally consists of a pure solvent such as deionized water

[SOURCE: OIML R 100-1:2013, 3.3.1]

3.4.3

blank value

reading or result originating from the *matrix* (3.3.9), reagents and any residual *bias* (3.8.5) in the measurement device or process, which contributes to the value obtained for the quantity in the analytical procedure

[SOURCE: PAC, 1989, 61, 1657 (Nomenclature for automated and mechanised analysis (Recommendations 1989))]

3.4.4

bracketing technique

analytical method consisting of bracketing the measured absorption or machine reading of the sample between two measurements made on *calibration solutions* (3.4.8) of neighbouring concentrations within the optimum working range

[SOURCE: ISO 6486-2:1999, 3.3]

3.4.5

calibration

operation that, under specified conditions, in a first step, establishes a relation between the *quantity values* (3.4.16) with measurement uncertainties provided by measurement standards and corresponding indications with associated *measurement uncertainties* (3.8.20) and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication

Note 1 to entry: A calibration can be expressed by a statement, calibration function, calibration diagram, *calibration curve* (3.4.7), or calibration table. In some cases, it can consist of an additive or multiplicative correction of the indication with associated *measurement uncertainty* (3.8.20).

Note 2 to entry: Calibration should not be confused with adjustment of a measuring system, often mistakenly called “self-calibration”, nor with *verification* (3.8.47) of calibration.

[SOURCE: ISO/IEC Guide 99:2007, 2.39]

3.4.6
calibration blank solution

solution prepared in the same way as the *calibration solution* (3.4.8) but leaving out the *analyte* (3.3.2), also called “zero member” of the *calibration* (3.4.5) series

[SOURCE: ISO 21400:2018, 3.8, modified]

3.4.7
calibration curve

expression of the relation between indication and corresponding *measured quantity value* (3.4.16.2)

Note 1 to entry: A calibration curve expresses a one-to-one relation that does not supply a measurement result as it bears no information about the *measurement uncertainty* (3.8.20).

[SOURCE: ISO/IEC Guide 99:2007, 4.31]

3.4.8
calibration solution

solution used to calibrate the instrument, prepared from a *stock solution* (3.4.21) or a certified standard by adding acids, *buffer* (3.6.5), *reference element* (3.7.7) and salts as needed

[SOURCE: ISO 21400:2018, 3.9]

3.4.9
certified reference material

CRM

reference material (RM) characterized by a metrologically valid procedure for one or more specified properties, accompanied by an RM certificate that provides the value of the specified property, its associated *uncertainty* (3.8.20), and a statement of metrological traceability

Note 1 to entry: The concept of value includes a nominal property or a qualitative attribute such as identity or sequence. Uncertainties for such attributes can be expressed as probabilities or levels of confidence.

[SOURCE: ISO Guide 30:2015, 2.1.2, modified — Notes 2, 3 and 4 to entry deleted.]

3.4.10
internal standard

compound added to a sample in a fixed amount that has similar properties (spectral, physical, isobaric etc.) to the target *analyte* (3.3.2) used to correct for instrument *drift* (3.6.15) and *matrix interference* (3.7.11)

[SOURCE: ISO/TS 20593:2017, 3.6, modified]

3.4.11
internal standard line

spectral line (3.6.40) of an *internal standard* (3.4.10), to which the radiant energy of an analytical line is compared

[SOURCE: ASTM E135:2021]

3.4.12
matrix solution

synthetic solution consisting of the solvent and containing, if possible, all the constituents of the *analytical sample* (3.3.3) except the *analyte* (3.3.2)

3.4.13

primary reference material

primary RM

high purity material of the *analyte* (3.3.2), certified for the mass/mole fraction of the *analyte* (3.3.2) in the material, and which constitutes the realization of the International System of Units (SI) for the *analyte* (3.3.2) of interest

Note 1 to entry: A primary reference material has its value assigned either directly by a primary RMP or indirectly by determining the impurities of the material by appropriate analytical methods (e.g. mass balance method).

[SOURCE: ISO 17511:2020, 3.35]

3.4.14

reference material

RM

material, sufficiently homogeneous and stable with respect to one or more specified properties, which has been established to be fit for its intended use in a measurement process

Note 1 to entry: RM is a generic term.

Note 2 to entry: Properties can be quantitative or qualitative, e.g. identity of substances or species.

Note 3 to entry: Uses can include the *calibration* (3.4.5) of a measurement system, assessment of a measurement procedure, assigning values to other materials, and *quality control* (3.8.26).

Note 4 to entry: ISO/IEC Guide 99:2007, 5.13 has an analogous definition, but restricts the term "measurement" to apply to quantitative values. However, Note 3 of ISO/IEC Guide 99:2007, 5.13, specifically includes qualitative properties, called "nominal properties".

[SOURCE: ISO/Guide 30:2015, 2.1.1]

3.4.15

reference method

reference measurement procedure

measurement procedure accepted as providing measurement results fit for their intended use in assessing *measurement trueness* (3.8.46) of *measured quantity values* (3.4.16.2) obtained from other measurement procedures for quantities of the same kind, in *calibration* (3.4.5), or in characterizing *reference materials* (3.4.14)

Note 1 to entry: The *accuracy* (3.8.1) of a reference method must be demonstrated through direct comparison with a definitive method or with a *primary Reference Material* (3.4.13).

[SOURCE: ISO/IEC Guide 99:2007, 2.7, modified — New preferred term added, Note to entry added.]

3.4.16

quantity value

number and reference together expressing magnitude of a quantity

[SOURCE: JCGM 200:2012 1.19]

3.4.16.1

reference quantity value

reference value

quantity value (3.4.16) used as a basis for comparison with values of quantities of the same kind

Note 1 to entry: A reference quantity value can be a *true quantity value* (3.8.45) of a measurand, in which case it is unknown, or a conventional quantity value, in which case it is known.

Note 2 to entry: A reference quantity value with associated *measurement uncertainty* (3.8.20) is usually provided with reference to:

a) a material, e.g. a *certified reference material* (3.4.9);

b) a device, e.g. a stabilized laser;

c) a *reference measurement procedure* (3.4.15);

d) a comparison of measurement standards.

[SOURCE: JCGM 200:2012, 5.18]

3.4.16.2
measured quantity value
value of a measured quantity
measured value
quantity value (3.4.16) representing a measurement result

[SOURCE: JCGM 200:2012, 2.10]

3.4.17
reference standard solution
solution containing an accurately known concentration of a sample element or elements of interest and that is used for testing and calibrating the instrument

[SOURCE: OIML R 100-1:2013, 3.4]

3.4.18
spike
known quantity of determinand that is added to a sample, usually for the purpose of estimating the *systematic error* (3.8.44) of an analytical system by means of a recovery exercise

Note 1 to entry: "Spiking" is a way of creating a *control material* (3.8.8) in which a value is assigned by a combination of formulation and analysis. This method is feasible when a test material essentially free of the *analyte* (3.3.2) is available. After exhaustive analytical checks to ensure the background level is adequately low, the material is spiked with a known amount of *analyte* (3.3.2). The reference sample prepared in this way is thus of the same *matrix* (3.3.9) as the test materials to be analysed and of known *analyte* (3.3.2) level - the *uncertainty* (3.8.20) in the assigned concentration is limited only by the possible *error* (3.8.11) in the unspiked determination. However, it can be difficult to ensure that the speciation, binding and physical form of the added *analyte* (3.3.2) is the same as that of the native *analyte* (3.3.2) and that the mixing is adequate.

[SOURCE: ISO 5667-14:2014, 3.7, modified — Note to entry added.]

3.4.19
standardization
process of adjusting instrument output to a previously established *calibration* (3.4.5) (that is, *drift correction* (3.6.16)); the experimental establishment of the concentration of a reagent solution

[SOURCE: ASTM E135: 2021]

3.4.20
standard solution
solution of accurately known concentration of an element, an ion, a compound or a group derived from the substance used for its preparation

Note 1 to entry: Standard solutions are prepared using standard substances in one of several ways. A primary standard is a substance of known high purity, which can be dissolved in a known volume of solvent to give a primary standard solution. If stoichiometry is used to establish the strength of a titrant, it is called a secondary standard solution. The term secondary standard can also be applied to a substance whose active agent contents have been found by comparison against a primary standard.

[SOURCE: ISO 78-2:1999, 3.6, modified — Note to entry added.]

3.4.21

stock solution

solution with accurately known *analyte* (3.3.2) concentration(s), prepared from pure chemicals such as a primary standard

[SOURCE: ISO 21400:2018, 3.11]

3.4.22

titration curve

plot of a variable related to a relevant concentration (activity) as the ordinate versus some measure of the amount of titrant, usually titration volume (titre), as the abscissa

Note 1 to entry: If the variable is linearly related to concentrations, such as the electrical conductance or the photometric absorbance, the expression "linear titration curve" is used. When a logarithmic expression of the concentration or activity is used, such as the pH, pM, or the electrical potential in mV, the curve is referred to as a logarithmic titration curve.

[SOURCE: IUPAC orange book:2002]

3.4.23

working reference materials

reference materials (3.4.14) used for routine analytical control and traceable to NIST standards and other recognized standards when appropriate standards are available

[SOURCE: ASTM A751:2020, 3.2.6]

3.4.24

working standard solution

solution, prepared by dilution of the stock standard solution(s), that contains the *analyte(s)* (3.3.2) of interest at a concentration(s) better suited to preparation of *calibration solutions* (3.4.8) than the concentration(s) of the *analyte(s)* (3.3.2) in the stock standard solution(s)

[SOURCE: ISO 15202-3:2004, 3.2.13]

3.5 Definitions of the analysis methods and analytical instrument

3.5.1

atomic absorption spectrometry

AAS

spectroanalytical method for qualitative determination and quantitative evaluation of element concentrations wherein the technique determines these concentrations by measuring the atomic absorption of free atoms

Note 1 to entry: The technique of analysis by AAS falls into two main categories, according to the method of atomization, that is, *flame atomic absorption spectrometry (FAAS)* (3.5.6) and *electrothermal atomic absorption (ETAAS)* (3.5.5) [also called graphite furnace atomic absorption spectrometry (GFAAS)].

[SOURCE: ISO 6486-1:2019, 3.2, modified — Note to entry added.]

3.5.2

atomic emission spectrometry

AES

pertaining to emission spectrometry in the ultraviolet, visible, or *infrared* (3.5.16) wavelength regions of the electromagnetic spectrum

Note 1 to entry: Atomic emission *spectroscopy* (3.5.26) is considered mainly in the ultraviolet and visible regions of the spectrum, i.e. the optical range, and makes use of different sampling sources that give rise to the different categories of *optical emission spectroscopy (OES)* (3.5.20), including flame, *plasma* (3.6.32), glow discharge, spark, direct current arc *optical emission spectroscopy* (3.5.20).

[SOURCE: ASTM E135:2021, modified — Note to entry added.]

3.5.3
atomic fluorescence spectrometry

AFS

method of determining chemical elements based on the measurement of the re-emission of characteristic electromagnetic radiation by atoms, following the absorption of radiation in the vapour phase

Note 1 to entry: The wavelengths of the absorbed and re-emitted radiation can be identical (atomic resonance fluorescence spectrometry) or different.

3.5.4
chemical vapour generation system

analyte (3.3.2) is separated from the sample *matrix* (3.3.9) by the generation of gaseous species as a result of a chemical reaction

Note 1 to entry: This technique has received its widest application in *atomic absorption spectrometry (AAS)* (3.5.1) in the forms of cold vapour AAS (CVAAS) for the determination of mercury and hydride generation AAS (HGAAS) for elements forming gaseous covalent hydrides (As, Bi, Ge, In, Pb, Sb, Se, Sn and Te). Chemical vapour generation is also used in combination with *optical emission* (3.5.20) and *atomic fluorescence spectrometry* (3.5.3).

[SOURCE: IUPAC orange book: 2002, 10.3.4.6]

3.5.4.1
cold vapour atomic absorption spectrometry

CVAAS

type of *atomic absorption spectrometry* (3.5.1) where no vaporisation step is required because the sample is a volatile heavy metal such as mercury, which is a vapour at room temperature

3.5.4.2
hydride generation atomic absorption spectrometry

HGAAS

type of *atomic absorption spectrometry* (3.5.1) where metal samples such as As, Sb and Se are vaporised by converting them into volatile hydrides

3.5.5
electrothermal atomic absorption spectrometry

ETAAS

type of spectrometry that uses a graphite-coated furnace to vaporize the sample

Note 1 to entry: This technique has largely been developed for use in *atomic absorption spectrometry* (3.5.1). It has also been applied in *atomic emission* (3.5.2) and *atomic fluorescence spectrometry* (3.5.3), with appropriate analogous phrases, such as electrothermal atomic emission spectrometry (ETAES) and electrothermal atomic fluorescence spectrometry (ETAFS).

3.5.6
flame atomic absorption spectrometry

measurement of the absorption of electromagnetic radiation, emitted by an element at a determined wavelength, by an absorbent medium (flame) formed of atoms of the same element that are in the ground state

Note 1 to entry: Each element absorbs radiation of specific wavelengths and the intensity of the absorbed radiation is proportional to the concentration of the said element.

[SOURCE: ISO 3750:2006, 3.1]

3.5.7
flame emission spectrometry

FES

chemical analysis method based on the measurement of light in a given range of wavelengths emitted by a sample atomized in a flame according to the Beer-Lambert law

Note 1 to entry: The functions of an analytical flame spectrometer in general are:

a) Transformation of the solution to be analyzed into a vapour containing free atoms or molecular compounds of the *analyte* (3.3.2) in the flame;

b) Selection and detection of the optical signal (arising from the *analyte* (3.3.2) vapour) which carries information on the kind and concentration of the *analyte* (3.3.2);

c) Amplification and read-out of the electrical signal.

[SOURCE: ISO 9555-3:1992, 3.1.6, modified — Note to entry added.]

3.5.8
Fourier transform infrared spectrometry

FT-IR spectrometry

form of infrared spectrometry in which an interferogram is obtained; which is then subjected to a Fourier transform to obtain an amplitude-wavenumber (or wave-length) spectrum

Note 1 to entry: The abbreviation FTIR is not recommended.

Note 2 to entry: When FT-IR spectrometers are interfaced with other instruments, a slash should be used to denote the interface; for example, GC/FT-IR; HPLC/FT-IR, and the use of FT-IR should be explicit, that is, FT-IR not IR.

[SOURCE: ASTM E131:2010]

3.5.9
glow discharge spectrometry

GDS

method in which a *spectrometer* (3.5.22) is used to measure relevant intensities emitted from a glow discharge generated at a surface

Note 1 to entry: This is a general term that encompasses GDOES and GDMS.

[SOURCE: ISO 18115-1:2013, 3.10]

3.5.10
glow discharge optical emission spectrometry

GDOES

method in which an optical emission spectrometer is used to measure the wavelength and intensity of light emitted from a glow *discharge* (3.6.14) generated at a surface

Note 1 to entry: This method is a spectroscopic method for the quantitative analysis of metals and other non-metallic solids. The metallic samples are used as a cathode in a direct current *plasma* (3.6.32). From the surface, the sample is removed in layers by sputtering with argon ions. The removed atoms pass into the *plasma* (3.6.32) by diffusion. Photons are emitted with excited waves and have characteristic wavelengths that are recorded by means of a downstream spectrometer and subsequently quantified. *Glow discharge spectroscopy* (3.5.9) is an established method for the characterization of *steels* (3.1.17) and varnishes.

[SOURCE: ISO 18115-1:2013, 3.9, modified — Note to entry added.]

3.5.11
gravimetry

set of methods used in analytical chemistry for the quantitative determination of an *analyte* (3.3.2) based on its mass

Note 1 to entry: The four main types of this method of analysis are precipitation, volatilization, electro-analytical and miscellaneous physical method. The methods involve changing the phase of the *analyte* (3.3.2) to separate it in its pure form from the original mixture and are quantitative measurements.

3.5.12
inductively coupled plasma

ICP

high-temperature *discharge* (3.6.14) generated in flowing argon by an alternating magnetic field induced by a radio frequency (RF) load coil that surrounds the tube carrying the gas

Note 1 to entry: In inductively coupled plasmas (inductively coupled RF plasmas or inductively coupled argon plasmas), energy transfer to the gas is achieved with the help of an induction coil or inductor (the terms coil, load coil and work coil are discouraged). The frequency at which the source operates should be given, e.g. 27 or 12 MHz, and the gas type should be defined. The *plasma* (3.6.32) is formed within and/or above a set of refractory tubes arranged coaxially with the induction coil, the whole forming a plasma torch.

[SOURCE: ISO 30011:2010, 3.3.5, modified — Note to entry added.]

3.5.13
inductively coupled plasma optical emission spectrometry

ICP-OES

measurement of the intensity of electromagnetic radiation emitted by the components of a sample when excited by a *plasma* (3.6.32)

Note 1 to entry: Sample atoms entering the plasma emit light radiation, whose characteristic wavelengths and intensities are used to identify the elements and determine concentrations, respectively. Samples are usually presented to the *plasma* (3.6.32) in solution form.

[SOURCE: ISO 3815-2:2005, 3.1]

3.5.14
inductively coupled plasma mass spectrometry

ICP-MS

analytical technique comprising a sample introduction system, an *inductively coupled plasma* (3.5.12) source for ionization of the *analytes* (3.3.2), a plasma/vacuum interface and a mass spectrometer comprising an ion focusing, separation and detection system

[SOURCE: ISO/TS 80004-6:2021, 5.23]

3.5.15
ion-selective electrode

ISE

potentiometric probe, the output potential of which, when measured against a suitable reference electrode, is proportional to the activity of the selected ion in the solution under test

Note 1 to entry: This is an electrochemical sensor, based on a thin selective membrane or film as recognition element and is an electrochemical half-cell equivalent to other half-cells of the zeroth (inert metal in a redox electrolyte), 1st, 2nd and 3rd kinds. These devices are distinct for half-cells that involve electrode redox reactions (electrodes of zeroth, 1st, 2nd and 3rd kinds), although they often contain a second kind electrode as the “inner” or “internal” reference electrode. The potential difference is the response (i.e. that of ISE versus outer reference electrode potentials) as its principal component of the Gibbs energy change associated with permselective mass transfer of ions (e.g. by ion-exchange, solvent extraction or some other mechanism) across a phase boundary. The ISE shall be used in conjunction with a reference electrode (i.e. “outer” or “external” reference electrode) to form a complete electrochemical cell. The measured potential difference s (ISE versus outer reference electrode potentials) are linearly dependent on the logarithm of the activity of a given ion in solution. The expression "ion-specific electrode" is not recommended. "Specific" implies that the electrode does not respond to additional ions. Since no electrode is truly specific for one ion, "ion-selective" is recommended as more appropriate. "Selective ion-sensitive electrode" is rarely used to describe an ion-selective electrode. "Principal" or "primary" ions are those for determination of which an electrode is designed. It is never certain that the ISE is more sensitive to the "principal" ion than to interferences, e.g. nitrate ISEs.

[SOURCE: 8.3.2.1, IUPAC orange book:2002]

3.5.16
infrared radiation
IR
infrared
optical radiation for which the wavelengths are longer than those for visible radiation

Note 1 to entry: For infrared radiation, the range between 780 nm and 1 mm is commonly subdivided into

- IR-A: 780 nm to 1 400 nm,
- IR-B: 1,4 µm to 3 µm, and
- IR-C: 3 µm to 1 mm.

Note 2 to entry: The range of infrared emitted by the source and which reaches the lens should be considered in the design of an infrared-absorbing material.

[SOURCE: IEC 60050-845:2020, 845-21-004, modified — Notes to entry delete, new Note 2 to entry added, "infrared" added as a preferred term.]

3.5.16.1
infrared spectroscopy
infrared (3.5.16) vibrational spectra originate in transitions between discrete vibrational energy levels of molecules, energy being absorbed from the incident *infrared* (3.5.16) beam by these transitions

Note 1 to entry: An absorption band is thus manifested as a reduction in the energy transmitted in the absence of the absorbing substance. The frequency of the absorption band can be related to the atomic masses and force constants of the vibrating molecule.

3.5.17
laser ablation inductively coupled plasma
laser ablation ICP
technique in which a laser beam focuses on the sample surface to erode material and generate fine particles

Note 1 to entry: The ablated particles are then transported to the secondary excitation source of the *inductively coupled plasma mass spectrometry (ICP-MS)* (3.5.14) instrument for digestion and ionization of the sampled mass. The excited ions in the plasma torch are subsequently introduced to a mass spectrometer detector for both elemental and isotopic analysis.

3.5.18
melt extraction
rapid quenching process in which the molten metal is brought into contact with the periphery of a rotating heat-extracting disk

Note 1 to entry: Quench rates exceed 1,000,000 K per second or process to “solidify rapidly” and extract a ribbon-like alloy product by the insertion of a short segment of a rotating chilled block into a bath of a molten metal alloy.

3.5.19
molecular absorption spectrophotometry
area concerned with the measured absorption of radiation in its passage through a gas, a liquid or a solid

Note 1 to entry: Molecules which absorb photons of energy corresponding to wavelengths in the range 190 nm to about 1000 nm exhibit UV /VIS absorption spectra.

Note 2 to entry: The UV/VIS absorption spectrum of a molecular species is normally represented as a graph of some characteristic for the radiation absorbed as a function of wavelength. The graph is representative for that species, solvent, concentration and temperature.

[SOURCE: IUPAC Manual of Symbols and Terminology, Part Vii: Molecular Absorption Spectroscopy, Ultraviolet And Visible (UV/VIS) (Recommendations 1988)]

3.5.20
optical emission spectrometry

measurement of the intensity of electromagnetic radiation emitted by the components of a sample when excited

Note 1 to entry: Each element emits radiation of well- defined and specific wavelength, whose intensity is linked to its concentration.

[SOURCE: ISO 3815-1:2005, 3.1]

3.5.20.1
arc emission spectrometry

spectrometry (3.5.26) where the sample is electrically conductive and can be used directly as one (or both) of the electrodes (self-electrode)

Note 1 to entry: For electrically non-conductive samples, powders or liquids, the sample is introduced into the different types of *discharge* (3.6.14) in a sample electrode, generally of graphite or amorphous carbon. The non-sample-carrying electrode is called the *counter electrode* (3.6.11) and can be of carbon, graphite or metal. Graphite and carbon electrodes differ in their electrical and thermal conductivity. The characteristics and operation of the arc depend on the material and shape of the electrodes and on the analytical gap (arc gap) as well as on the polarity of the sample electrode. If the sample electrode is positive, anodic vaporization takes place. If the sample electrode is negative, cathodic vaporization ensues. If radiation from only a thin layer near the cathode is utilized, the technique is known as the cathode layer arc.

[SOURCE: IUPAC orange book:2002, 10.3.4.1]

3.5.20.2
spark emission spectrometry

spectrometry (3.5.26) where spark sources, because of their relatively high *precision* (3.8.22) and *accuracy* (3.8.1), are suitable sources for the routine analysis of metals, e.g. for production control purposes

Note 1 to entry: Metals can be analysed with the point-to-point configuration using two sample electrodes (self-electrodes) of the same material. The most common technique uses the point-to-plane configuration, i.e. a plane electrode made from the sample material with a pointed *counter electrode* (3.6.11) made from another material, which does not contain the analytical elements. Various types of samples can be analysed in the form of solutions with the help of supporting electrodes (e.g. copper spark and graphite spark supporting electrode techniques), carrier electrodes, rotating disc or rotating platform electrodes, vacuum cup or porous cup electrodes.

[SOURCE: IUPAC orange book:2002, 10.3.4.2]

3.5.21
potentiometry

measure of the potential difference between an indicator electrode and a reference electrode (or another indicator electrode) in solution, while the current is held at zero, because no faradaic current flows, the potential is usually controlled by the thermodynamic properties of the system

Note 1 to entry: The expressions “zero current potentiometry” and “null-current potentiometry” are not recommended. No special terminology is recommended for measurements of pH and similar quantities.

[SOURCE: IUPAC orange book:2002, 8.5]

3.5.22
spectrometer

spectral apparatus for measuring the intensity of one or more spectral bands as a function of a spectral variable

3.5.23
sequential spectrometer

spectrometer (3.5.22) that enables the intensity of several spectral bands of radiation to be measured one after the other in time, i.e. sequentially

[SOURCE: IUPAC orange book:2002, 10.3.2.1.2]

3.5.24
simultaneous spectrometer

spectrometer (3.5.22) with more than one detector that enables the intensities of several spectral bands to be measured at the same time

[SOURCE: IUPAC orange book:2002, 10.3.2.1.2]

3.5.25
spectrochemical analysis

process in which a sample is submitted to a procedure in which its constituents emit or absorb radiation

Note 1 to entry: Radiation is generated by radiation sources. The element sought or determined in a sample is the *analyte* (3.3.2). It is characterized by a specific absorption or emission that is related to its quantity or concentration in the sample.

[SOURCE: IUPAC orange book: 2002, 10.2]

3.5.26
spectroscopy

study of physical systems by the electromagnetic radiation with which they interact or that they produce

Note 1 to entry: In certain types of optical spectroscopy, the radiation originates from an external source and is modified by the system, whereas in other types, the radiation originates within the system itself.

[SOURCE: PAC, 1986, 58, 1737 (Quantities and units in clinical chemistry: Nebulizer and flame properties in flame emission and absorption spectrometry (Recommendations 1986))]

3.5.27
spectrophotometer

optical instrument that measures spectral transmittance or reflectance

Note 1 to entry: This instrument consists of an optical source, a monochromator, a sample chamber, an optical detector, a signal processor, a data processor and an interface

3.5.28
thermal conductometry

measurement of a sample gas is a method of determining the gas concentrations of binary mixtures by utilizing the difference of thermal conductivities between two gas components

Note 1 to entry: Current, traditional katharometer technologies not only measure the thermal conductivity but also the thermal mass of the gas thus causing distortion to the measurement.

3.5.29
titration

quantitative chemical analysis to determine the concentration of an identified *analyte* (3.3.2)

Note 1 to entry: Process of determining the quantity of a substance: A, by adding measured *increments* (3.3.6) of substance B, with which it reacts (almost always as a standardized solution called the titrant, but also by electrolytic generation, as in coulometric titration) with provision for some means of recognizing (indicating) the point, the end point at which essentially all of A has reacted.

3.5.30
X-ray fluorescence

emission of characteristic X-radiation by an atom as a result of the interaction of electromagnetic radiation with its orbital electrons

[SOURCE: PAC, 1994, 66, 2513 (Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994))]

3.5.31

X-ray fluorescence analysis

method of analysis based on the measurement of the energies and intensities of characteristic X-radiation emitted by a *test portion* (3.3.14) during irradiation with X-rays of wavelength shorter than their characteristic wavelengths

[SOURCE: IUPAC orange book: 2002, 16]

3.5.31.1

energy dispersive X-ray fluorescence analysis

method of *X-ray fluorescence analysis* (3.5.31) where element specificity is obtained by measuring the energy spectrum of the induced X-radiation

[SOURCE: PAC, 1982, 54, 1533 (Glossary of terms used in nuclear analytical chemistry (Provisional))]

3.6 Definitions relating to characteristics and properties of the equipment

3.6.1

absorption path length

length of the radiation path through the absorbing medium equal to the cell path length, l, in the case of single-pass cells at normal incidence of radiation

[SOURCE: IUPAC orange book: 2002]

3.6.2

absorbance matching

procedure where the concentration of a known *analyte* (3.3.2) is determined by diluting the sample with solvent until the absorbance matches the absorbance of a known concentration of the *analyte* (3.3.2) in the reference cell

Note 1 to entry: This method is particularly useful if the Beer-Lambert law does not hold.

[SOURCE: IUPAC orange book:2002, 10.3.5.2.7]

3.6.3

axial plasma

end-on plasma

plasma (3.6.32) that is viewed end-on by the optical detection system

[SOURCE: ISO 15202-3:2004, 3.3.1]

3.6.4

background radiation

radiation from any source other than the one it is desired to detect or measure

[SOURCE: PAC, 1994, 66, 2513 (Nomenclature for radioanalytical chemistry (IUPAC Recommendations 1994)) Orange Book]

3.6.5

buffer

substance that tends to minimize the effects of one or more elements on the emission of other elements

[SOURCE: ASTM E135:2021, modified — Note 1 to entry added.]

3.6.6

characteristic concentration

characteristic mass

concentration or mass of an element that produces a change from the *blank test solution* (3.4.1) of 0,004 4 absorbance units (1 % absorption) at the wavelength of the absorption line employed

[SOURCE: OIML R 100-1:2013]

3.6.7
characteristic line

line used for the measurement of *analyte* (3.3.2) concentration by flame atomic emission, absorption or fluorescence in the vapour phase

Note 1 to entry: Characteristic lines include resonance and other lines.

3.6.8
charge-coupled device detector

CCD

type of solid state detector technology for converting photons into an electrical signal

Note 1 to entry: Typically applied to inductively coupled plasma-optical emission spectroscopy (ICP-OES).

3.6.9
charge-injection device detector

CID

type of solid state detector technology for converting photons into an electrical signal

Note 1 to entry: Typically applied to inductively coupled plasma-optical emission spectroscopy (ICP-OES).

3.6.10
collimator

device made from radiation absorbent material such as lead or tungsten, designed to limit and define the direction and area of the radiation beam

[SOURCE: ISO 5576:1997, 2.21]

3.6.11
counter electrode

auxiliary electrode

electrode commonly used in applied polarization to balance the current passing to the working electrode

Note 1 to entry: It is usually made from a non-corroding material.

[SOURCE: ISO 8044:2020, 7.1.39]

3.6.12
direct-injection burner

combines the function of *nebulizer* (3.6.30) and burner

Note 1 to entry: Here, oxidant and fuel emerge from separate ports and are mixed above the burner orifices to produce a turbulent flame. Most commonly, the oxidant is also used for aspirating and nebulizing the sample. However, when the fuel is used for this purpose, the expression "reversed direct-injection burner" is applied. In each case, the mist droplets enter the flame directly, without passing through a *spray chamber* (3.6.41).

Note 2 to entry: The expression "total-consumption burner", which is often used, is not recommended.

[SOURCE: IUPAC orange book: 2002, 10.3.4.3]

3.6.13
D_2-lamp

hydrogen (discharge) lamp filled with dideuterium in place of dihydrogen

Note 1 to entry: This substitution increases the intensity 3-to 5-fold for the same power consumption and extends the upper limit of the continuum further into the visible range.

3.6.14
discharge
triggered capacitor
series of electrical discharges from capacitors initiated by a separate means and extinguished when the voltage across the analytical gap falls to a value that no longer is sufficient to maintain it

[SOURCE: ASTM E135:2021]

3.6.15
drift
slow change of a metrological characteristic of a measuring instrument

3.6.16
drift correction
process of adjusting for a translational shift or a rotational shift, or both, in an instrument *calibration* (3.4.5)

[SOURCE: ASTM E135:2021]

3.6.17
efficiency of nebulization
ε_n
ratio of the amount of *analyte* (3.3.2) entering the flame to the amount of *analyte* (3.3.2) aspirated

Note 1 to entry: The quantity, ε_n, is not related to the amount of solvent but to the amount of *analyte* (3.3.2). Its value cannot be determined unambiguously by simply comparing the volume of solution drained per second from the *spray chamber* (3.6.41) with the aspiration rate. Correction is usually made for the difference in *analyte* (3.3.2) concentration in the drained and aspirated solutions respectively, due to the partial evaporation of solvent from the mist droplets deposited on the walls. The quantity, ε_n is not merely characteristic of the operation of the *nebulizer* (3.6.30) but of the nebulizer-burner system as a whole.

[SOURCE: IUPAC orange book: 2002, 10.3.4.3]

3.6.18
electrothermal atomizer
device that is heated to the temperature required for *analyte* (3.3.2) atomization, by the passage of electrical current through its body

Note 1 to entry: This technique has largely been developed for use in *atomic absorption spectrometry* (3.5.1). It has also been applied in *atomic emission* (3.5.2) and *atomic fluorescence spectrometry* (3.5.3). See *electrothermal atomic absorption spectrometry* (3.5.5).

[SOURCE: IUPAC orange book:2002, 10.3.4.5]

3.6.19
electrodeless discharge lamp
EDL
glass tube filled with an excitable substance and sealed under a reduced pressure or a noble gas, a high frequency electromagnetic field (radio frequency or MW, 300 MHz to 3 000 MHz) can trigger gas *discharge* (3.6.14) causing the emission of electromagnetic radiation

Note 1 to entry: This phenomenon has been studied for many years and was already well understood in the 1960s. EDL is usually characterized by a higher emission intensity than that of the *hollow cathode lamps* (3.6.24), a lower contamination due to the absence of the electrodes, and a longer lifetime. EDLs operate due to free electrons in the fill that are accelerated by the MW field energy. They collide with the gas atoms and ionize them to release more electrons (the “avalanche” effect). The energetic electrons collide with the heavy-atom particles present in the *plasma* (3.6.32), thus exciting them from the ground state to higher energy levels. The *excitation energy* (3.6.20) is then released as the electromagnetic radiation with the spectral characteristics according to the composition of the fill.

3.6.20
excitation energy
minimum energy required to bring a system to a specified higher energy level

[SOURCE: IUPAC Orange Book, 223]

3.6.21
fuel-lean flame
burning of fuel with an excess of air in an internal combustion engine

Note 1 to entry: In lean-burn engines the air, fuel ratio can be as lean as 65:1 (by mass)

3.6.22
fuel-rich flame
mixture of fuel and air, in which the fuel content is greater than that of a stoichiometric mixture

Note 1 to entry: to promote the atomization of elements that readily form oxides in the vapour phase in the flame, a fuel-rich flame is often chosen, where reducing conditions favour the dissociation of metal oxides

3.6.23
high voltage sparks
self-ignited spark *discharge* (3.6.14) characterized by an initial capacitor voltage exceeding the breakdown voltage of the analytical gap or of the control gap

Note 1 to entry: Typical capacitor voltages range from 10 to 20 kV.

[SOURCE: IUPAC orange book: 2002, 10.3.1.3]

3.6.24
hollow cathode source
hollow cathode lamp
HCL
discharge lamp designed for use as a *spectral line* (3.6.40) source with atomic absorption (AA) *spectrometers* (3.5.22)

Note 1 to entry: A single or multi-element hollow cathode lamp is required for each element to be determined using the AA technique.

Note 2 to entry: The key requirement for the hollow cathode lamp is to generate a narrow emission line for the element being determined. The emission line should be of sufficient spectral purity and intensity to achieve a good *calibration* (3.4.5) (preferably linear) with low noise.

3.6.25
infrared detector
sensor that converts absorbed *infrared radiation* (3.5.16) into an electrical signal

Note 1 to entry: The two main types of detectors are thermal and photonic (photodetectors).

[SOURCE: ISO 10878:2013, 1.51, modified — Note to entry added.]

3.6.26
instrumental drift
continuous or incremental change over time in indication, due to changes in metrological properties of a measuring instrument

Note 1 to entry: Instrumental drift is related neither to a change in a quantity being measured nor to a change of any recognized influence quantity physical interferences.

[SOURCE: JCGM 200:2012, 4.21]

3.6.27
ionization efficiency
ratio of the number of ions formed to the number of electrons, ions, or photons used in an ionization process

[SOURCE: ISO 18115-1:2013, 4.273]

3.6.28
inductively coupled plasma torch
ICP torch
device used to support and introduce sample into an ICP discharge

Note 1 to entry: An ICP torch usually consists of three concentric tubes, the outer two usually made from quartz.

[SOURCE: ISO 15202-3:2004, 3.3.6]

3.6.29
linear dispersion
derivative, $dx/d\lambda$, where x is the distance along the spectrum, in the plane of the exit slit, and λ is the wavelength

[SOURCE: ASTM E131:2010]

3.6.30
nebulizer
device for converting a sample solution into a gas-liquid aerosol for atomic absorption, emission, fluorescence, or mass analysis

[SOURCE: ASTM E135:2021]

3.6.30.1
pneumatic nebulizer
nebulizer (3.6.30) that uses high-speed gas flows to create an aerosol from a liquid

[SOURCE: ISO 15202-3:2004, 3.3.19]

3.6.30.2
ultrasonic nebulizer
nebulizer (3.6.30) in which the aerosol is created by flowing a liquid across a surface that is oscillating at an ultrasonic frequency

[SOURCE: ISO 15202-3:2004, 3.3.24]

3.6.31
photomultiplier tube
electronic device for amplifying and converting light pulses into measurable electrical signals

Note 1 to entry: Vacuum phototube with additional amplification by electron multiplication. It consists of a photocathode, a series of dynodes, called a dynode chain on which a secondary-electron multiplication process occurs, and an anode. According to the desired response time, transit time, time spread, gain, or low dark current, different types of dynode structures have been developed, e.g. circular cage structure, linear focused structure, venetian blind structure, box and grid structure. Some special dynode structures permit combination with additional electric or magnetic fields. A strip dynode photomultiplier tube consists of a photocathode followed by thin dynode material on an insulating substrate. In a continuous-strip photomultiplier, two strip dynodes are arranged in parallel. A potential applied to the ends of the two strips produces an electric field across the continuous strip dynodes, giving rise to electron multiplication along the dynodes. In a resistance-strip magnetic photomultiplier, a uniform magnetic field is applied to the planes of the strips so that the electrons travel in the crossed electric and magnetic fields. A channel photomultiplier tube photocathode consists of a channel electron multiplier (CEM) system for the photoelectrons and an anode to collect the final electron current. The basic part of the CEM is a tube with a semiconducting inner surface. In general, it is curved in order to inhibit the acceleration of positive ions towards the photocathode. A number of small channels called micro channels can be constructed in arrays for imaging applications.

[SOURCE: PAC, 1995, 67, 1745 (Nomenclature, symbols, units and their usage in spectrochemical analysis-XI. Detection of radiation (IUPAC Recommendations 1995))]

3.6.32
plasma
gas that is at least partly ionized and contains particles of various type, that is, electrons, atoms, ions and molecules

Note 1 to entry: Plasma as a whole is electrically neutral

[SOURCE: IUPAC orange book:2002,10.3.1.1.1]

3.6.33
pre-burn period
time interval after the initiation of a *discharge* (3.6.14) during which the emitted radiation energy is not recorded for analytical purposes

[SOURCE: ASTM E135:2021]

3.6.34
premix burner
burner in which the fuel gas is mixed with the oxidizing gas before reaching the combustion zone

[SOURCE: ASTM E135:2021]

3.6.35
primary X-rays
emergent beam from the X-ray source

[SOURCE: ASTM E135:2021]

3.6.36
radial plasma
plasma (3.6.32) that is viewed from the side by the optical detection system

[SOURCE: ISO 15202-3:2004, 3.3.20]

3.6.37
reciprocal linear dispersion
derivative $d\lambda/dx$ where λ is the wavelength and x is the distance along the spectrum

[SOURCE: ASTM E135:2021]

3.6.38
secondary fluorescence
ionization of the *analyte* (3.3.2) element in a sample by characteristic radiation from other elements in the sample resulting in an enhancement of the signal measured

[SOURCE: PAC, 1980, 52, 2541 (Nomenclature, symbols, units and their usage in spectrochemical analysis – IV X-ray emission spectroscopy)]

3.6.39
spectral slit width
mechanical width of the exit slit, divided by the *linear dispersion* (3.6.29) in the exit slit plane spark

[SOURCE: ASTM E131:2010]

3.6.40
spectral line
atomic and ionic spectral lines originate from specified electronic transitions between energy levels of atoms and ions, respectively

Note 1 to entry: In the past, it has been common usage to denote atomic lines as arc lines and ionic lines as spark lines. This usage is now considered to be incorrect. The correct way to indicate that lines are due to atomic or ionic transitions is: Element symbol I wavelength, e.g. Cu I 324,7 nm; and Element symbol II wavelength, e.g. Cu II 213,6 nm. Similarly, for higher states of ionization, the type of line is represented by III, IV, etc.

[SOURCE: IUPAC orange Book, 118]

3.6.41
spray chamber
device, placed between a *nebulizer* (3.6.30) and an *inductively coupled plasma (ICP) torch* (3.6.28), whose function is to separate out aerosol droplets according to their size, so that only very fine droplets pass into the *plasma* (3.6.32) and large droplets are drained or pumped to waste

[SOURCE: ISO 15202-3:2004, 3.3.21]

3.6.42
viewing height
observation height
position in a *radial plasma* (3.6.36) from where the emission measured originates

Note 1 to entry: The viewing height is generally given as the distance, in millimetres, above the load coil.

[SOURCE: ISO 15202-3:2004, 3.3.25]

3.6.43
zeeman effect
splitting or shift of *spectral lines* (3.6.40) due to the presence of an external magnetic field

[SOURCE: PAC, 1996, 68, 2223 (Glossary of terms used in photochemistry (IUPAC Recommendations 1996)) 2284 Orange Book]

3.7 Definitions relating to interference

3.7.1
background correction
process of correcting the intensity at an analytical wavelength for the intensity due to the underlying *spectral background* (3.7.19)

[SOURCE: ISO 15202-3:2004, 3.3.2]

3.7.2
excitation interference
matrix interference (3.7.11) that manifests itself as a change in *sensitivity* (3.8.36) due to a change in *plasma* (3.6.32) conditions when the *matrix* (3.3.9) of a *calibration* (3.4.5) or *test solution* (3.3.16) is introduced into the *plasma* (3.6.32)

[SOURCE: ISO 15202-3:2004, 3.3.5]

3.7.3
inter-element correction
interference correction
spectral interference correction technique in which emission contributions from interfering elements that emit at the *analyte* (3.3.2) wavelength are subtracted from the apparent *analyte* (3.3.2) emission after measuring the interfering element concentrations at other wavelengths

[SOURCE: ISO 15202-3:2004, 3.3.10]

3.7.4

interfering lines

radiation from nearby *spectral lines* (3.6.40) may perturb the measurement of the intensity of the line wanted, these lines are termed interfering lines

[SOURCE: IUPAC Orange Book, 159]

3.7.5

interfering substance

(in electroanalytical chemistry) substance, other than the ion being measured, whose presence in the sample solution affects the measured emf of a cell

Note 1 to entry: Interfering substances fall into two classes: 'electrode/electrochemical' interferences and 'chemical' interferences. Examples of the first class include:

a) Those substances which give a similar response to the ion being measured and whose presence generally results in an apparent increase in the activity (or concentration) of the ion to be determined (e.g. Na +for the Ca2+ electrode).

b) Electrolytes present at a high concentration that give rise to appreciable liquid junction potential differences or results in a significant activity coefficient decrease, or incipient Donnan exclusion failure. The second class of substances that should be recognized as chemical interferences includes:

c) Species that interact with the ion being measured so as to decrease its activity or apparent concentration. The electrode continues to report the true activity (e.g. CN –present in the measurement of Ag+), but a considerable gap will occur between the activity and concentration of the ions even in very dilute solutions. Under these circumstances the determination of ionic concentration may be problematic.

d) Substances interacting with the membrane itself, blocking the surface or changing its chemical composition [i.e. organic solvents for the liquid or poly(vinyl chloride) (PVC) membrane electrodes] are grouped as interferences or electrode poisons.

[SOURCE: PAC, 1994, 66, 2527(Recommendations for nomenclature of ion-selective electrodes (IUPAC Recommendations 1994))]

3.7.6

interference reduction

techniques used to reduce or eliminate analytical *errors* (3.8.11) resulting from various types of interferences apart from changing the instrumental conditions

Note 1 to entry: Some of those in current use are given in 3.7.6.1 to 3.7.6.4.

3.7.6.1

reference-element technique

technique where the measure of the *analyte* (3.3.2) is compared with the measure of a *reference element* (3.7.7)

Note 1 to entry: This technique is used mainly for minimizing nonspecific interferences.

3.7.6.2

analyte addition technique

technique where *errors* (3.8.11) arising from both specific and non-specific interferences, but not from *spectral interferences* (3.7.18), are minimized

3.7.6.3

simulation technique

technique where reference solutions sufficiently similar in quantitative composition to the sample solutions to be analysed are used so that the interferences in the reference and sample solution are equivalent

3.7.6.4

buffer-addition technique

technique where an additive [called a *spectrochemical buffer* (3.7.17)] is added to both the sample and reference solutions for the purpose of making the measure of the *analyte* (3.3.2) less sensitive to variations in interferent concentration

3.7.7

internal standardization

reference element

technique that uses the signal from *an internal standard* (3.4.10) to correct for *matrix interferences* (3.7.11)

3.7.8

isobaric overlap

basic spectral overlap between *analyte* (3.3.2) ions

Note 1 to entry: An isobaric overlap exists where two elements have isotopes of essentially the same mass. It is notable that there are no isobaric interferences below 36 m/z.

3.7.9

masking reagent

substance that decreases the concentration of a free metal ion or ligand by conversion into an essentially unreactive form, thus preventing undesirable chemical reactions that would interfere with the determination

3.7.10

matrix effect

composite interference due to all the concomitants, except for the additives

[SOURCE: 10.3.4.3, IUPAC orange book:2002]

3.7.11

matrix interference

non-spectral interference

interference of a non-spectral nature caused by a difference between the *matrix* (3.3.9) of the *calibration* (3.4.5) and *test solutions* (3.3.16)

3.7.12

matrix-matching

technique used to minimize the effect of *matrix interferences* (3.7.11) on analytical results, involving the preparation of *calibration solutions* (3.4.8) in which the concentrations of acids and other major solutes are matched with those in the *test solutions* (3.3.16)

[SOURCE: ISO 15202-3:2004, 3.3.16]

3.7.13

pyrolytic techniques

techniques used for the high-temperature thermal decomposition of a *test sample* (3.3.15) or for its conversion from one chemical form to another

Note 1 to entry: Although not primarily intended as a method of pre-concentration, pyrolytic techniques can be used to separate the *analyte* (3.3.2) or analytes from the *matrix* (3.3.9) of the *test sample* (3.3.15). In a technique called furnace pyrolysis, a flowing stream of gas (hydrogen, oxygen, nitrogen, chlorine, etc.) required to produce volatile species of the elements being determined, is passed over the *test sample* (3.3.15) in a heated furnace. The *analytes* (3.3.2) leave the furnace in the gas stream or are entrained by a carrier gas. The *analytes* (3.3.2) in the gas stream can be collected in an absorbing solution, on a carbon or other filter or by condensation on a cool surface. In the case of mercury, this can also be done by amalgamation with a noble metal. The *analytes* (3.3.2) can then be swept and released from the trap, by heating, into a sampling source for analysis. The *test sample* (3.3.15) can also be mixed with a reagent to produce a volatile compound which is volatilized by heating and separated by distillation. Metallic samples can be dissolved by anodic oxidation. This technique can also be used to oxidize and dissolve inclusions or base metal phases from metals and alloys.

[SOURCE: IUPAC orange book: 2002, 10.3.4.9]

3.7.14
self-absorption
event that occurs in emission sources of finite thickness when radiant energy quanta emitted by atoms (or molecules) are absorbed by atoms of the same kind present in the same source

Note 1 to entry: The absorbed energy is usually dissipated by collisional transfer of energy or through emission of radiant energy of the same or other frequencies. In consequence, the observed radiant intensity of a *spectral line* (3.6.40) (or band component) emitted by a source can be less than the radiant intensity would be from an optically thin source having the same number of emitting atoms. Self-absorption can occur in all emitting sources to some degree, whether they are homogeneous or not.

[SOURCE: Orange Book, 242 PAC, 1996, 68, 2223 (Glossary of terms used in photochemistry (IUPAC Recommendations 1996))]

3.7.15
spectrochemical additive
additive that is added to samples and reference samples with the intention of making the measure of the analytical element less sensitive to changes in concentration of an interferent

[SOURCE: IUPAC orange book: 2002, 10.3.4.1.6]

3.7.15.1
spectrochemical diluent
substance added to the sample to increase its bulk for ease of handling or for the suppression of undesirable *matrix effects* (3.7.10)

[SOURCE: IUPAC orange book: 2002, 10.3.4.1.6]

3.7.15.2
spectrochemical carrier
additive that gives rise to a gas that can help to transport the vapour of the sample material into the excitation region of the source

[SOURCE: IUPAC orange book: 2002, 10.3.4.1.6]

3.7.16
solute-volatilization interference
interference that is due to changes in the volatilization rate of the dry aerosol particles in the case when volatilization of the *analyte* (3.3.2) is incomplete in the presence and/or absence of the concomitant

Note 1 to entry: These interferences can either be specific, if the *analyte* (3.3.2) and interferent form a new phase of different thermostability, as when Mg and Al form MgAl2O4 in an air-acetylene flame, or non-specific, if the *analyte* (3.3.2) is simply dispersed in a large excess of the interferent, as when Ag is dispersed in ThO2. Solute volatilization interferences do not necessarily depress the signal. Effects due to compounds causing explosive disintegration of the solid aerosol particles and consequent enhancement also belong to this group.

[SOURCE: IUPAC orange book: 2002, 10.3.4.3]

3.7.17
spectrochemical buffer
buffer with the intention of making the measure of the analytical element less sensitive to changes in concentration of an interferent

Note 1 to entry: Additives that can serve as spectrochemical buffers are given in 3.7.17.1 to 3.7.17.6.

3.7.17.1
suppressor
additive that reduces emission, absorption or light scattering by an interferent, thus removing or lowering spectral interference

3.7.17.2
releaser

additive that reduces *solute-volatilization interferences* (3.7.16) by forming a compound preferentially with the interferent, thus preventing the reaction of the *analyte* (3.3.2) or interferent from entering a thermally stable compound

3.7.17.3
ionization buffer

additive that are added to increase the free-electron concentration in the flame gases, thus repressing and stabilizing the degree of ionization

3.7.17.4
volatilizer

additive that increase the fraction volatilized, either by forming more volatile compounds or by increasing the total surface area of all *analyte* (3.3.2) particles [e.g. by explosive disintegration or by dispersal of the *analyte* (3.3.2) in a highly volatile *matrix* (3.3.9)]

3.7.17.5
devolatilizer

material added to a sample to reduce its volatilization, or that of some component of it

Note 1 to entry: A typical devolatilizer is carbon, which gives rise to refractory carbides when used in the analysis of tungsten or boron.

3.7.17.6
saturator

interferent added in sufficiently high concentration to the sample solution to reach the saturation plateau of the interference curve

[SOURCE: IUPAC orange book: 2002, 10.3.4.3]

3.7.18
spectral interference

incomplete isolation of the radiation emitted or absorbed by the *analyte* (3.3.2) from other radiation detected by the instrument

Note 1 to entry: Spectral interferences are usually strongly dependent on the spectral bandwidth of the monochromator. Spectral interferences can arise:

a) In *flame emission spectrometry (FES)* (3.5.7) from the following:

   - radiation [spectral continuum, molecular bands, or atomic lines (called *interfering lines* (3.7.4))] emitted by the concomitants. Spectral interference can also arise from stray or scattered radiation or spectral ghosts that reach the detector or from the indirect effect of the concomitants on flame background.

b) In *flame atomic absorption spectrometry (FAAS)* (3.5.6) and/or flame atomic fluorescence spectrometry (FAFS) by the following:

   - absorption or fluorescence of radiation by overlapping molecular or atomic lines of concomitants;
   - thermal emission of concomitants transmitted by the monochromator or received;
   - the photodetector as stray radiation, when the radiation source is not modulated;
   - scattering of source radiation by non-volatilized particles formed by the concomitants;
   - the indirect effect of the concomitants on the blank background absorption or scattering in the flame;
   - foreign line absorption and/or fluorescence if the corresponding radiation happens to be emitted by the light source, in addition to the analysis line, within the spectral bandwidth of the monochromator, particularly when a continuum source is used.

Note 2 to entry: Spectral interferences on inductively coupled plasma-optical emission spectroscopy (ICP-OES) occur either on the analytic signal or on the *background correction* (3.7.1) points for the signal; stray light from the line emission of high concentration elements; overlap of a *spectral line* (3.6.40) from another elements; or unresolved overlap of molecular band spectra.

[SOURCE: IUPAC orange book: 2002, 10.3.4.3]

3.7.19
spectral background
intensity that would be measured at the wavelength or energy of the *analyte* (3.3.2) line if the *analyte* (3.3.2) and overlapping lines were not present

[SOURCE: ASTM E135:2021]

3.7.20
spectral background correction
spectral background (3.7.19) absorbance of a sample arising, for example, from the presence of an impurity with a weak, broad absorption band, which can be made by subtracting it from the *analyte* (3.3.2) absorbance by graphical or algebraic methods

[SOURCE: IUPAC orange book: 2002, 10.3.5.2.3]

3.7.21
titration error
difference in the amount of titrant, or the corresponding difference in the amount of substance being titrated, represented by the expression: (End-point value) - (Equivalent-point value)

[SOURCE: IUPAC orange book:2002]

3.7.22
vapour-phase interferences
change in the fraction of *analyte* (3.3.2) *dissociated* (3.7.23), ionized or excited in the gaseous phase

Note 1 to entry: The word "atomized" (instead than "dissociated") is not appropriate here because the latter also covers the formation of free atomic ions. These interferences can be called dissociation, ionization, and *excitation interferences* (3.7.2), respectively. An *excitation interference* (3.7.2) can occur when the concomitant alters the flame temperature. Experimentally these interferences can be easily recognized because they take place even when twin *nebulizers* (3.6.30) are used for aspirating the *analyte* (3.3.2) and interferent separately. All interferences of this type are specific.

[SOURCE: IUPAC orange book: 2002, 10.3.4.3]

3.7.23
dissociated
formed of free neutral atoms from free molecules in the gaseous phase

3.8 Characteristics of methods

3.8.1
accuracy
accuracy of measurement
measurement accuracy
closeness of agreement between a *measured quantity value* (3.4.16.2) and a *true quantity value* (3.8.45) of a measurand

Note 1 to entry: The concept "measurement accuracy" is not a quantity and is not given a numerical quantity value. A measurement is said to be more accurate when it offers a smaller *measurement error* (3.8.11).

Note 2 to entry: The term "measurement accuracy" should not be used for *measurement trueness* (3.8.46) and the term "*measurement precision* (3.8.22)" should not be used for "measurement accuracy", which, however, is related to both these concepts.

Note 3 to entry: "Measurement accuracy" is sometimes under-stood as closeness of agreement between measured quantity values that are being attributed to the measurand.

[SOURCE: ISO/IEC Guide 99:2007, 2.13]

3.8.2
arithmetic mean
average
$\overline{x}$ sum of a series of observations divided by the number of observations calculated by the following formula: $\overline{x} = \frac{\sum x_\mathrm{i}}{n}$ where

x_i is the individual value of a parameter with $i = 1, 2, 3 \ldots n$;

n is the number of observations.

Note 1 to entry: All summations are taken from 1 to n. The arithmetic mean is an unbiased estimate of the population mean, i.e. μ is the limiting value for $\overline{x}_i$,as $n \to \infty$.

[SOURCE: PAC, 1994, 66, 595 (Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))]

3.8.3
background equivalent concentration
BEC
elemental concentration required to produce an *analyte* (3.3.2) signal with the same intensity as a background signal

[SOURCE: ISO 11885:2007, 3.3]

3.8.4
between-laboratory standard deviation
standard deviation (3.8.42) of results obtained on the same material using the same method in different laboratories

[SOURCE: ASTM E135: 2021]

3.8.5
bias
measurement bias
estimate of a *systematic measurement error* (3.8.44)

[SOURCE: ISO/IEC Guide 99:2007, 2.18]

3.8.6
confidence level
confidence coefficient
value $(1 - \alpha)$ of the probability associated with a confidence interval or a statistical coverage interval

Note 1 to entry: $(1 - \alpha)$ is often expressed as a percentage.

Note 2 to entry: In some cases, the confidence level is dictated by the needs of the situation. In all other instances, use of $1\text{-}\alpha = 0{,}95$ is recommended.

3.8.7
control chart
chart with control limits on which some statistical measure of a series of samples is plotted in a particular order to steer the process with respect to that measure

Note 1 to entry: The particular order is usually based on time or sample number order.

Note 2 to entry: The control chart operates most effectively when the measure is a process variable that is correlated with an ultimate product or service characteristic.

[SOURCE: ISO 3534-2:2006, 2.3.1, modified]

3.8.7.1
Shewhart control chart

control chart (3.8.7) with Shewhart control limits intended primarily to distinguish between the variation in the plotted measure due to random causes and that due to special causes

Note 1 to entry: This can be a chart using attributes (for example, proportion nonconforming) for evaluating a process, or it can be a chart using variables (for example, average and range) for evaluating a process. Examples are as follows:

a) X-bar chart — the sample means are plotted in order to control the mean value of a variable;

b) R chart — the sample ranges are plotted in order to control the variability of a variable;

c) s chart — the sample *standard deviations* (3.8.42) are plotted in order to control the variability of a variable;

d) s^2 chart — the sample variances are plotted in order to control the variability of a variable;

e) C chart — the number of defectives (per batch, per day, per machine, etc.) is plotted.

[SOURCE: ISO 3534-2:2006, 2.3.2, modified — Note 1 to entry added.]

3.8.8
control material

material used for the purposes of internal *quality control* (3.8.26) and subjected to the same or part of the same measurement procedure as that used for test materials

Note 1 to entry: Note to 1 entry: *Reference materials* (3.4.14) can be used as control material, ideal control materials are the certified ones.

[SOURCE: IUPAC orange book: 2002, 18.6.1]

3.8.9
degrees of freedom

statistical quantity indicating the number of values which could be arbitrarily assigned within the specification of a system of observations.

Note 1 to entry: For simple replication, with n measurements and one estimated parameter (the mean), $v=n-1$. More generally, for multivariable computations, the number of degrees of freedom equals the number of observations minus the number of fitted parameters

[SOURCE: PAC, 1994, 66, 595 (Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))]

3.8.10
deviation

d_i

difference between an observed value and the *arithmetic mean* (3.8.2) of the set to which it belongs calculated by the following formula:

$$d_i = x_i - \bar{x}$$

where

x_i is an observed value;

$\bar{x}$ is the arithmetic mean of the set.

[SOURCE: PAC, 1994, 66, 595 (Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994))]

3.8.11
error

error of measurement

measurement error

measured quantity value (3.4.16.2) minus a *reference quantity value* (3.4.16.1)

Note 1 to entry: The concept of "measurement error" can be used both

a) when there is a single reference quantity value to refer to, which occurs if a *calibration* (3.4.5) is made by means of a measurement standard with a measured quantity value having a negligible *measurement uncertainty* (3.8.20) or if a conventional quantity value is given, in which case the measurement error is known, and

b) if a measurand is supposed to be represented by a unique *true quantity value* (3.8.45) or a set of true quantity values of negligible range, in which case the measurement error is not known.

Note 2 to entry: Measurement error should not be confused with production error or mistake.

[SOURCE: ISO/IEC Guide 99:2007, 2.16]

3.8.12
instrumental bias

average (3.8.2) of replicate indications minus a *reference quantity value* (3.4.16.1)

[SOURCE: JCGM 200:2012, 4.20]

3.8.13
intralaboratory comparison

organization, performance and evaluation of measurements or tests on the same or similar items within the same laboratory in accordance with predetermined conditions

[SOURCE: ISO/IEC 17025:2017, 3.4]

3.8.14
intermediate precision condition of measurement

intermediate precision condition

condition of measurement, out of a set of conditions that includes the same measurement procedure, same location, and replicate measurements on the same or similar objects over an extended period of time, but may include other conditions involving changes

Note 1 to entry: The changes can include new *calibrations* (3.4.5), calibrators, operators, and measuring systems.

Note 2 to entry: A specification for the conditions should contain the conditions changed and unchanged, to the extent practical.

Note 3 to entry: In chemistry, “inter-serial precision condition of measurement” is sometimes used to designate this concept.

[SOURCE: ISO/IEC Guide 99:2007, 2.22]

3.8.15
intermediate measurement precision

intermediate precision

measurement precision (3.8.22) under a set of intermediate precision conditions of measurement

Note 1 to entry: Relevant statistical terms are given in ISO 5725-3.

[SOURCE: ISO/IEC Guide 99:2007, 2.23]

3.8.16
limit of detection
LOD
detection limit
DL
measured quantity value (3.4.16.2), obtained by a given measurement procedure, for which the probability of falsely claiming the absence of a component in a material is β, given a probability α of falsely claiming its presence

Note 1 to entry: IUPAC recommends default values for α and β equal to 0,05.

Note 2 to entry: The term "*sensitivity* (3.8.36)" is discouraged for 'detection limit'.

Note 3 to entry: The limit of detection shall be calculated as:

$$X_{LD} = 3s$$

where

X_{LD} is the limit of detection;

s is the *standard deviation* (3.8.42) of the outlier-free results of at least 3 measurements of a reagent blank solution).

[SOURCE: ISO/IEC Guide 99:2007, 4.18, modified — Note 2 to entry deleted, new Note 3 to entry added.]

3.8.17
limit of quantification
quantification limit
LOQ
lowest amount of an *analyte* (3.3.2) that is quantifiable with a given *confidence level* (3.8.6)

Note 1 to entry: The limit of quantification can be calculated as ten times the *standard deviation* (3.8.42) of blank measurements.

Note 2 to entry: The value LOQ can be used as a threshold value to assure quantitative measurement of an *analyte* (3.3.2) accurately.

[SOURCE: ISO 18158:2016, 2.4.3.5]

3.8.18
linearity
straight line relationship between the (mean) result of measurement (signal) and the quantity (concentration) of the component to be determined

[SOURCE: ISO 11885:2007, 3.9]

3.8.19
long-term stability
stability (3.8.39) of a *reference material* (3.4.14) property over an extended period of time

[SOURCE: ISO Guide 30:2015, 2.1.17]

3.8.20
measurement uncertainty
uncertainty of measurement
uncertainty
non-negative parameter characterizing the dispersion of the *quantity values* (3.4.16) being attributed to a measurand, based on the information used

Note 1 to entry: Measurement uncertainty includes components arising from systematic effects, such as components associated with corrections and the assigned quantity values of measurement standards, as well as the definitional uncertainty. Sometimes estimated systematic effects are not corrected for but, instead, associated measurement uncertainty components are incorporated.

Note 2 to entry: The parameter can be, for example, a *standard deviation* (3.8.42) called standard measurement uncertainty (or a specified multiple of it), or the half-width of an interval, having a stated coverage probability.

Note 3 to entry: Measurement uncertainty comprises, in general, many components. Some of these can be evaluated by Type A evaluation of measurement uncertainty from the statistical distribution of the quantity values from series of measurements and can be characterized by *standard deviations* (3.8.42). The other components, which can be evaluated by Type B evaluation of measurement uncertainty, can also be characterized by *standard deviations* (3.8.42), evaluated from probability density functions based on experience or other information.

Note 4 to entry: In general, for a given set of information, it is understood that the measurement uncertainty is associated with a stated *quantity value* (3.4.16) attributed to the measurand. A modification of this value results in a modification of the associated uncertainty.

[SOURCE: ISO/IEC Guide 99: 2007, 2.26]

3.8.21
minimum standard deviation
standard deviation (3.8.42) of results on a test material obtained under conditions of minimum variability

[SOURCE: ASTM E135:2021]

3.8.22
measurement precision
precision
closeness of agreement between indications or *measured quantity values* (3.4.16.2) obtained by replicate measurements on the same or similar objects under specified conditions

Note 1 to entry: Measurement precision is usually expressed numerically by measures of imprecision, such as *standard deviation* (3.8.42), variance or coefficient of variation under the specified conditions of measurement.

Note 2 to entry: The 'specified conditions' can be, for example, *repeatability conditions of measurement* (3.8.33.1), *intermediate precision conditions of measurement* (3.8.14), or *reproducibility conditions of measurement* (3.8.34.1) (see ISO 5725-1:1994).

Note 3 to entry: Measurement precision is used to define *measurement repeatability* (3.8.33), *intermediate measurement precision* (3.8.15), and *measurement reproducibility* (3.8.34).

Note 4 to entry: Sometimes "measurement precision" is erroneously used to mean measurement *accuracy* (3.8.1).

[SOURCE: ISO/IEC Guide 99:2007, 2.15]

3.8.23
outlier
member of a set of values which is inconsistent with the other members of that set

Note 1 to entry: ISO 5725-2 specifies the statistical tests and the significance level to be used to identify outliers in *trueness* (3.8.46) and *precision* (3.8.22) experiments.

[SOURCE: ISO 5725-1:1994, 3.21]

3.8.24
photometric linearity
ability of a photometric system to yield a linear relationship between the radiant power incident on its detector and some measurable quantity provided by the system

Note 1 to entry: In the case of a simple detector-amplifier combination, the relationship is a direct proportionality between incident radiant power and the deflection of a meter needle or recorder pen.

[SOURCE: ASTM E131:2010]

3.8.25
quality assurance
part of quality management focused on providing confidence that quality requirements will be fulfilled

[SOURCE: ISO 9000:2015, 3.3.6]

3.8.26
quality control
part of quality management focused on fulfilling quality requirements

[SOURCE: ISO 9000:2015, 3.3.7]

3.8.27
random measurement error
random error of measurement
random error
component of *measurement error* (3.8.11) that in replicate measurements varies in an unpredictable manner

Note 1 to entry: A *reference quantity value* (3.4.16.1) for a random measurement error is the average that would ensue from an infinite number of replicate measurements of the same measurand.

Note 2 to entry: Random measurement errors of a set of replicate measurements form a distribution that can be summarized by its expectation, which is generally assumed to be zero, and its variance.

Note 3 to entry: Random measurement error equals measurement error minus systematic measurement error.

[SOURCE: ISO/IEC Guide 99:2007, 2.19]

3.8.28
random fluctuations
random errors (3.8.27) limiting the *precision* (3.8.22) of analysis

Note 1 to entry: When measuring very large or very small absorbances, uncertainties due to random fluctuations become particularly large. To obtain better *precision* (3.8.22) in the absorption measurement, it is necessary to adjust the sample concentration or cell path length to bring the absorbance into the range 0,1 to 1,0. The theoretical minimum *error* (3.8.11) occurs at a best *precision* (3.8.22) absorbance of about 0,43 for a *spectrometer* (3.5.22) with a detector that is thermal noise limited, e.g. phototube or photodiode, and of about 0,86 for a *spectrometer* (3.5.22) with a detector that is shot noise limited, e.g. a *photomultiplier* (3.6.31).

[SOURCE: IUPAC orange book:2002, 10.3.5.2.8]

3.8.29
regression analysis
use of statistical methods for modeling a set of dependent variables, *Y*, in terms of combinations of predictions, *X*

Note 1 to entry: It includes methods such as multiple linear regression (MLR) and partial least squares (PLS).

[SOURCE: PAC, 1997, 69, 1137 (Glossary of terms used in computational drug design (IUPAC Recommendations 1997))]

3.8.30
relative standard deviation

s_r

standard deviation (3.8.42) divided by the mean of the series calculated with the following:

$$s_r = \frac{s}{\bar{x}}$$

where

s is positive square root of the variance

$\bar{x}$ is the mean of the series

Note 1 to entry: sigma (σ) and 's' as representing the *standard deviation* (3.8.42) of a normal distribution is simply that sigma (σ) signifies the idealised population *standard deviation* (3.8.42) derived from an infinite number of measurements, whereas 's' represents the sample *standard deviation* (3.8.42) derived from a finite number.

[SOURCE: PAC, 1994, 66, 595 (Nomenclature for the presentation of results of chemical analysis (IUPAC Recommendations 1994)) Orange Book]

3.8.31
relative detection limit

smallest amount of material detectable (3σ-criterion) in a *matrix* (3.3.9) relative to the amount of material analysed, given in atomic, mole or weight fractions

Note 1 to entry: Often incorrectly referred to as "sensitivity" (3.8.36).

[SOURCE: PAC, 1979, 51, 2243 (General aspects of trace analytical methods - IV. Recommendations for nomenclature, standard procedures and reporting of experimental data for surface analysis techniques)]

3.8.32
relative standard measurement uncertainty

standard measurement uncertainty divided by the absolute value of the *measured quantity value* (3.4.16.2)

[SOURCE: ISO/IEC Guide 99:2007, 2.32]

3.8.33
repeatability

measurement repeatability

measurement precision (3.8.22) under a set of repeatability conditions of measurement

[SOURCE: ISO/IEC Guide 99:2007, 2.21]

3.8.33.1
repeatability condition of measurement

repeatability condition

condition of measurement out of a set of conditions that includes the same measurement procedure, same operators, same measuring system, same operating conditions and same location, and replicate measurements on the same or similar objects over a short period of time

Note 1 to entry: In chemistry, the expression “intra-serial precision condition of measurement” is sometimes used to designate this concept.

[SOURCE: ISO/IEC Guide 99:2007, 2.20]

3.8.33.2
repeatability limit

r

value less than or equal to which the absolute difference between two test results obtained under *repeatability conditions* (3.8.33.1) can be expected to be with probability of 95 %

[SOURCE: ISO 5725-1: 1994, 3.16]

3.8.33.3
repeatability standard deviation

standard deviation (3.8.42) of test results or measurement results obtained under *repeatability conditions* (3.8.33.1)

Note 1 to entry: It is a measure of the dispersion of the distribution of test or measurement results under *repeatability conditions* (3.8.33.1).

Note 2 to entry: Similarly, “repeatability variance” and “repeatability coefficient of variation” can be defined and used as measures of the dispersion of test or measurement results under *repeatability conditions* (3.8.33.1).

[SOURCE: ISO 3534-2:2006, 3.3.7]

3.8.33.4
repeatability relative standard deviation

RSD_r

measure used to show the extent of variability in relation to the mean of the population

Note 1 to entry: *Relative standard deviation (RSD)* (3.8.30) is a useful measure of *precision* (3.8.22) in quantitative studies and reflects *precision* (3.8.22) under *repeatability conditions* (3.8.33.1). The RSD is also known as coefficient of variation.

3.8.34
reproducibility

measurement reproducibility

measurement precision (3.8.22) under reproducibility conditions of measurement

Note 1 to entry: Relevant statistical terms are given in ISO 5725-1:1994 and ISO 5725-2:2019.

[SOURCE: ISO/IEC Guide 99: 2007, 2.25]

3.8.34.1
reproducibility condition of measurement

reproducibility condition

condition of measurement, out of a set of conditions that includes different locations, operators, measuring systems, and replicate measurements on the same or similar objects

Note 1 to entry: The different measuring systems can use different measurement procedures.

Note 2 to entry: A specification should give the conditions changed and unchanged, to the extent practical.

[SOURCE: ISO/IEC Guide 99: 2007, 2.24]

3.8.34.2
reproducibility limit

R

value less than or equal to which the absolute difference between two test results obtained under *reproducibility conditions* (3.8.34.1) can be expected to be with probability of 95 %

[SOURCE: ISO 5725-1:1994, 3.20]

3.8.34.3
reproducibility standard deviation

standard deviation (3.8.42) of test results or measurement results obtained under *reproducibility conditions* (3.8.34.1)

Note 1 to entry: It is a measure of the dispersion of the distribution of test or measurement results under *reproducibility conditions* (3.8.34.1).

Note 2 to entry: Similarly, "reproducibility variance" and "reproducibility coefficient of variation" can be defined and used as measures of the dispersion of test or measurement results under *reproducibility conditions* (3.8.34.1).

[SOURCE: ISO 3534-2:2006, 3.3.12]

3.8.35
resolution

smallest change in a quantity being measured that causes a perceptible change in the corresponding indication

Note 1 to entry: Resolution can depend on, for example, noise (internal or external) or friction. It can also depend on the value of a quantity being measured.

[SOURCE: ISO/IEC Guide 99: 2007, 4.14]

3.8.36
sensitivity

slope (3.8.41) of the *calibration curve* (3.4.7)

Note 1 to entry: If the curve is a curve, rather than a straight line, then of course sensitivity will be a function of *analyte* (3.3.2) concentration or amount.

Note 2 to entry: If sensitivity is to be a unique performance characteristic, it must depend only on the chemical measurement process, not upon scale factors.

[SOURCE: PAC, 1995, 67, 1699 (Nomenclature in evaluation of analytical methods including detection and quantification capabilities (IUPAC Recommendations 1995))]

3.8.37
sensitivity of a measuring system

quotient of the change in an indication of a measuring system and the corresponding change in a value of a quantity being measured

Note 1 to entry: Sensitivity of a measuring system can depend on the value of the quantity being measured.

Note 2 to entry: The change considered in a value of a quantity being measured must be large compared with the *resolution* (3.8.35).

[SOURCE: ISO/IEC Guide 99: 2007, 4.12]

3.8.38
selectivity
selectivity of a measuring system

property of a measuring system, used with a specified measurement procedure, whereby it provides *measured quantity values* (3.4.16.2) for one or more measurands such that the values of each measurand are independent of other measurands or other quantities in the phenomenon, body, or substance being investigated

EXAMPLE 1 Capability of a measuring system including a mass spectrometer to measure the ion current ratio generated by two specified compounds without disturbance by other specified sources of electric current.

EXAMPLE 2 Capability of a measuring system to measure the power of a signal component at a given frequency without being disturbed by signal components or other signals at other frequencies.

EXAMPLE 3 Capability of a receiver to discriminate between a wanted signal and unwanted signals, often having frequencies slightly different from the frequency of the wanted signal.