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Metrological and quality concepts in analytical chemistry

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Metrological and Quality Concepts in Analytical Chemistry (IUPAC Provisional Recommendations 2020)

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Abstract: Recommendations are given for metrological terminology in analytical chemistry. Analytical chemistry is defined and concepts relating to laboratory practice are termed and defined. Recommendations are given concerning the terminology of quality assurance in analytical chemistry. Terms draw on the extensive quality literature, particularly from ISO.

Keywords: analytical chemistry, metrology, calibration, measurement, measurement uncertainty, quality assurance, quality control, validation, interlaboratory comparison, internal quality control, conformity assessment

This work was started under the project 2012-007-1-500: Metrology - IUPAC Orange Book Chapter 1, with membership of D. Brynn Hibbert and Paul De Bièvre (Task group Chairs), Peter Bode, René Dybkaer, Ernst-Heiner Korte, Pentti Minkinen, Jürgen Stohner, and Barry Wise. It has been completed by the authors of these Recommendations.

Dedication

Our good friend and colleague Paul De Bièvre, who died on 14 April 2016, was the 'father' of chemists' fundamental understanding of metrology. His outlook and wise suggestions permeate these Recommendations and they will be part of the legacy he has left to chemistry.

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René Dybkaer, who died on 29 April 2019, has also been an inspiration for these Recommendations on fundamental aspects of analytical chemistry. A stalwart of laboratory medicine and metrology he gave his advice to the authors freely and at length. We acknowledge his enormous contribution.

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INTRODUCTION

Metrology, being the science of measurement and its application, covers the experimental production and the use of quantity values in all disciplines of science and engineering, including chemistry and, not least, analytical chemistry. The metrological concepts to be applied in all sciences are defined in the 3rd edition of the International vocabulary of metrology - Basic and general concepts and associated terms (VIM) [1], however, the various disciplines have specialized tasks and typical laboratory procedures to meet the metrological challenges in their fields. This requires us to identify and define dedicated concepts to ensure consistent application and terminology and, therefore, these Recommendations aim at providing such concepts and terms to complement the VIM in the field of analytical chemistry. Hopefully, this will contribute to focusing their current usage and stabilizing their consistent application.

The VIM and present IUPAC format of a concept entry provides term(s), definition, and explanation by examples and notes, and in case the source. VIM entries will not be reproduced here, except where the original text (mostly notes and examples) is modified to suit the needs of analytical chemistry; in such a case "[VIM n.m]" (where n.m is the entry number) is given as source. For non-VIM concepts the respective reference number (e.g. [2] for ISO Guide 30) is used in the sense that information is taken from there. Within the entries, terms referring to concepts defined within these Recommendations or concepts defined in the VIM appear in italics on first use. VIM concepts are referenced with the VIM entry number e.g. *measurement unit* [VIM 1.9]. Note that terms originating in the VIM that are reproduced here with amendment are given in italics but not followed by the VIM reference denoting a cross reference within these Recommendations.

As in the VIM, commonly uses basic statistical terms are not referenced where they appear in individual entries. Most of these are defined in the three parts of ISO 3534 [3-5].

- population [3] entry 1.1
- probability (of an event) [3] entry 2.5
- statistic [3] entry 1.8
- standard deviation [3] entry 2.37
- variance [3] entry 2.36
- covariance [3] entry 2.43
- average, mean [3] entry 1.15
- median [3] entry 2.14
- mode [3] entry 2.27
- correlation coefficient [3] entry 2.44
- standard error [3] entry 1.24
- characteristic [4] entry 1.1.1
- action limit [4] entry 2.4.4
- warning limit [4] entry 2.4.3

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Compliance with the norms issued by JCGM, ISO, and IUPAC is intended. Regarding the not always uniform usage of some terms it should be noted that in the VIM, terms such as "length", "energy", "mass concentration" are used to identify both specific concepts under '*quantity*' [VIM 1.1] (Note 1) and *'kinds-of-quantity*' [VIM 1.2] (Note 3). While in laboratory medicine [6] these concepts are termed "kinds of quantity" throughout, we will follow the usage of the Green Book [7], the *International System of Quantities* (ISQ) [VIM 1.6] etc. to refer to them as "quantities".

These Recommendations result from updating the third edition of the Orange Book [8] and provide concepts for Chapters 1 and 13 in the forthcoming fourth edition, “Compendium of Terminology in Analytical Chemistry”.

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1 DEFINITION OF ANALYTICAL CHEMISTRY

1.1 analytical chemistry

Scientific discipline that develops and applies strategies, instruments, and procedures to obtain information on the composition and nature of matter in space and time.

Note 1: The definition was coined by the Working Party on Analytical Chemistry (WPAC) of the Federation of European Chemical Societies (FECS) and is known as the “Edinburgh Definition”. [9]

Note 2: The term ‘analytical science’ was coined [10] in 1998 to emphasize the impact of informatics on analytical chemistry.

Source: [9]. See also *chemical analysis*.

1.2 chemical analysis

Application of *analytical chemistry*.

Source: [9].

1.3 qualitative analysis

Examination [11] of *nominal properties* [VIM 1.30] in *analytical chemistry*.

Note 1: Qualitative analysis is used to detect and establish the identity of *chemical substances* and species.

Example: Identification of heroin (diacetylmorphine) in a *sample* of white powder seized by the police.

Note 2: Qualitative analysis should not be related to *ordinal quantity* [VIM 1.26] or *unitary quantity*.

1.4 quantitative analysis

Measurement in *analytical chemistry*.

Note: Quantitative analysis is used to obtain *quantity values* [VIM 1.19] for *ordinal quantities* [VIM 1.26] and *unitary quantities*.

Entry replaces recommendation in [12] p 1701.

2 CONCEPTS USED IN LABORATORY PRACTICE

2.5 additive matrix effect

Matrix effect that is independent of the *measured quantity value* [VIM 2.10] of the *measurand* [VIM 2.3].

Note 1: An additive matrix effect affects the intercept, not the slope of a linear *calibration curve*.

Note 2: The effect is sometimes termed “translational matrix effect” or “background interference” [13].

Example 1: An additive matrix effect that originates from a missing or flawed *blank correction*. [14]

Example 2: The measurement of plutonium mass concentration by a K-edge densitometer in the presence of a uranium admixture. The presence of uranium causes a large additive matrix effect. [15]

2.6 aliquot
specimen

Portion of a material assumed to be taken with negligible sampling error [16].

Example: An aliquot of an *analytical sample* is subjected to *chemical analysis* by chromatography.

Note 1: The concept is usually applied to fluids. It can also be used for sufficiently homogeneous solids such as powders. See *material homogeneity*.

Entry replaces recommendation in [17] p 1206. See also *sample*.

2.7 analyte

Component specified in a *measurand*.

Note 1: Analyte, or the name of a *chemical substance* or one of its *components*, are terms sometimes used for ‘measurand’. This usage is erroneous because these terms do not refer to *quantities* [VIM 1.1] as it is required for the concept 'measurand'. See also Note 4 to measurand.

Note 2: A component to be identified by examination [11] should not be termed analyte.

Entry replaces recommendation in [18] p 1660.

2.8 analytical function

See: *calibration curve*.

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2.9 analytical run
run

Set of *measurements* of the same *quantity* [VIM 1.1] performed under *repeatability conditions of measurement*.

Note: An analytical run may comprise measurements on one or more *reference materials*, *blank materials, quality control materials*, and *analytical samples*.

Source [19].

2.10 analytical sample

Sample, taken and, if need be, prepared from a *laboratory sample*, portions of which are subject to *chemical analysis*.

Note 1: The analytical sample may be considered to be the combination of an *analyte* and *matrix*.

Note 2: A portion of the analytical sample may be termed an *aliquot* if it is taken with negligible sampling error [16].

Source: [17].

2.11 background indication

Indication [VIM 4.1] obtained from a phenomenon, body, or substance similar to the one under investigation, but for which a *quantity* [VIM 1.1] of interest is supposed not to be present or is not contributing to the indication.

Source: [VIM 4.2].

Note: In VIM 4.2 this concept is termed “blank indication” with "background indication" as alternate term. However, since *blank indication* refers to the explicit use of a *blank material* in *analytical chemistry* it should be distinguished from the concept ‘background indication’.

Source: [8] p 44 of section 18.

2.12 batch

Material which is known or assumed to be produced under uniform conditions.

Note 1: Some vocabularies assume “*lot”* and “batch” to be synonymous. The distinction made here with respect to knowledge of production history permits a lot to consist of one or more batches and is useful in interpreting the results of *chemical analysis*.

Source: [17] entry 2.2.3.

2.13 blank correction

Step in a *measurement procedure* in which the effect of a *blank indication* is removed from an *indication* [VIM 4.1].

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Note 1: The blank indication and the indication must be of the same *kind of quantity* [VIM 1.2].

Note 2: A blank indication may be subtracted from an indication, or, in the case of a transmittance measurement, the indication is divided by the blank indication.

2.14 blank indication

Indication [VIM 4.1] obtained from a sample of *blank material* under the measurement conditions for the *measurand*.

Note: In VIM 4.2 “background indication” is given as an alternate term for blank indication. However, the terms refer to different concepts. [8] p 44 of section 18.

Entry replaces recommendation in [18] p 1662, [20] p 2167.

2.15 blank material
blank

Material which contains no, or as little as possible, of the *analyte* of interest, used in *measurement* to establish a *blank indication*.

Note 1: *Testing*, processing and measurement of blank materials are nearly always an essential part of *chemical analysis* and may be part of *quality assurance* and *quality control*. See [21].

Note 2: The concept may be extended to more than one analyte.

Note 3: Terms such as “solvent blank”, “reagent blank” or “matrix blank” are often used to specify the type of blank material.

Note 4: The term “procedure blank” is often used to denote a material that is carried through the entire *measurement procedure*. Terms such as “field blank”, “calibration blank” and “instrument blank” refer to materials handled in specific parts of the measurement procedure.

Note 5: A blank material to which a relevant *component* has been added is often termed “spiked blank” or “fortified blank”. Compare *spike*, *internal standard* and *measurement procedure with standard addition*.

Note 6: If the term "blank" is used, e.g. to denote blank indication or the related *blank value* or *blank correction*, this must be clarified by the context.

Source: [19, 21].

2.16 blank value

Measured quantity value [VIM 2.10] obtained by application of the *calibration function* to the *blank indication*.

Note: The concepts 'blank value' and *'blank indication*' should not be confused.

2.17 calibration certificate

Document issued by a technically competent *organization* providing information about a *calibration* [VIM 2.39].

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Note 1: The document may include a statement describing the calibration procedure and the *calibrators* [VIM 5.12] (calibrants) applied along with the *calibration curve*, *calibration diagram* [VIM 4.30] or other presentation of the calibration.

Note 2: Calibration certificates are often valid for a stated period of time, although this is not stipulated in ISO/IEC 17025 [22].

Note 3: The authority of the body issuing the document comes from its demonstrated technical *competence*.

2.18 calibration curve

Expression of the relation between *indication* [VIM 4.1] and corresponding *measured quantity value* [VIM 2.10].

Note 1: A calibration curve expresses a one-to-one relation that does not supply a *measurement result* [VIM 2.9] as it bears no information about the *measurement uncertainty* [VIM 2.26].

Source: [VIM 4.31].

Note 2: A calibration curve is usually shown in the form of a smooth curve interpolating the data points.

Note 3: The term “response curve” is sometimes used for a concept having the same or broader meaning.

Note 4: In the VIM *calibration diagram* [VIM 4.30] is defined as "Graphical expression of the relation between indication and corresponding measurement result". A calibration diagram allows measurement uncertainty to be represented in it, and so differs from a calibration curve.

2.19 calibration function

Presentation of *calibration curve* by a mathematical function.

Note 1: A calibration function is established by fitting a mathematical function to the data from the first step of *calibration* [VIM 2.39] using the measured quantity values provided by *measurement standards* [VIM 5.1] as input variables to calculate the expected indication. A calibration function bears no information about *measurement uncertainty* [VIM 2.26]. See also Note 1 to *linearity of calibration*; Note 2 to *measurement procedure with standard addition*.

Note 2: Mathematical analysis of the fit of a calibration function may give a contribution to an *uncertainty budget* [VIM 2.33] for a measured quantity value obtained from the calibration.

Note 3: The inverse of the calibration function, often termed "analytical function", is applied on an observed indication to attribute a measured quantity value. This corresponds to the second step described in the definition of calibration.

Entry replaces recommendation in [12] p 1703.

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2.20 calibration interval

Time period between *calibrations* [VIM 2.39] over which the performance of the *measuring system* [VIM 3.2] may be expected to meet specified *requirements*.

Note 1: Guidelines for the determination of calibration intervals of measuring systems are given in ILAC-G24 [23].

Note 2: ISO 14532 refers to a period "between routine calibrations" [24].

2.21 certified property value
certified value

Property value of a *reference material*, accompanied by statements of associated uncertainty and traceability, and identified as a certified property value in the *reference material certificate*.

Note: In this definition, "traceability" covers both *metrological traceability* [VIM 2.41] of a *measurement result* [VIM 2.9] and examination traceability [11] but not *object traceability*. Similarly "uncertainty" covers *measurement uncertainty* [VIM 2.26] and examination uncertainty [11].

Source: [2]. See also: *non-certified property value*.

2.22 chemical purity
purity

Mass (amount of substance, number of entities) of a specified *component* divided by the mass (amount of substance, number of entities, respectively) of the *system*.

Note 1: Purity is usually related to a major component. The other components are termed "impurities".

Note 2: The *quantity* [VIM 1.1], component and system must be specified.

Note 3: The *numerical quantity value* [VIM 1.20] of purity is often expressed as per cent or per mille.

Note 4: Purity can be estimated as $1-\sum_{j=1}^{j=N} f_j$ where f_j are fractions of the same type (mass fraction, amount of substance fraction) of all other components $j = 1, ..., N$. If the contributions are expressed as mass fractions, this estimation is sometimes termed "mass balance".

2.23 chemical substance
substance

Matter of constant composition best characterized by the entities (molecules, formula units, atoms) it is composed of.

Note: Physical *quantities* [VIM 1.1] such as density, refractive index, electrical conductivity, and melting point characterize a chemical substance.

Source: [25] entry C01039 (http://goldbook.iupac.org/terms/view/C01039).

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2.24 component

Part of a *system*.

Source: [26].

Note 1: A component may consist of different species.
Note 2: 'Part' is not to be taken for an *aliquot* or a portion or a *sample* of a system.

2.25 consensus property value
consensus value

Property value derived from a collection of results.

Note 1: The term “consensus value” is typically used to describe estimates of a measure of location, such as mean value, median or mode, and dispersion derived from results reported by *participants* in a *proficiency testing round*, but may also be used to refer to values derived from results of a specified subset of such results or, for example, from a number of laboratories chosen for their expertise for the particular analysis.

Source: [27].

Note 2: The consensus property value, when it is a value of a *unitary quantity*, may be expressed as a mean, median, or mode, and is then termed "consensus mean", "consensus median", or "consensus mode" respectively. The mode and the median also apply for *ordinal quantities* [VIM 1.26] and the mode for *nominal properties* [VIM 1.30].
Note 3: A consensus property value is an example of *assigned value*.
Note 4: A consensus property value could, through appropriate actions, become a *certified property value*; this is in analogy to the *certification of a reference material*.
Note 5: A consensus property value may be obtained in a material-certification study or by agreement between appropriate *organizations* or experts.

Source: [28, 29].

2.26 conventional quantity value
conventional value of a quantity
conventional value

Quantity value [VIM 1.19] attributed by agreement to a *quantity* [VIM 1.1] for a given purpose.

Example 3: Conventional quantity value of a given mass standard, m = 100.003 47 g.
Note 2: Sometimes a conventional quantity value is an estimate of a *true quantity value* [VIM 2.11].
Note 3: A conventional quantity value is generally accepted as being associated with a suitably small *measurement uncertainty* [VIM 2.26], which might be zero.

Source: [VIM 2.12] with Note 1 and Examples 1,2 omitted.

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Example 4: Relative atomic mass for carbon as listed in the IUPAC Green Book [7] p117.

Example 5: *Consensus property value* of the *measured values* [VIM 2.10] of an *interlaboratory comparison* [27].

Note 4: In *quality assurance* and *quality control* in chemistry a conventional quantity value, which may be a consensus property value, is often termed "*assigned value*".

2.27 critical value, L_c
critical level
decision level

Measured quantity value [VIM 2.10] for a *quantity* [VIM 1.1] of a *component* in a material above which the component is declared to be present.

Note 1: The critical value is usually considered to be a characteristic of a particular *measurement procedure*, performed in a particular laboratory.

Note 2: In some European legislation the term "decision level" (there denoted $CC\alpha$) is used for the concept 'critical value'[30].

Note 3: The quantity measured is usually a mass fraction or a concentration but can also be for example, a mass or amount of substance.

Note 4: The critical value is chosen to give a probability α (usually 0.05) of a measured quantity value exceeding the critical value when the component is absent.

Note 5: The detection decision is made by comparing a measured quantity value with the critical value.

Note 6: Another important concept in characterizing the *capability* of detection of measurement procedures is *limit of detection*.

Source: [12, 31].

2.28 determination

Set of operations that are carried out on an object in order to provide qualitative or quantitative information about this object.

Note 1: Determination is a term in general usage and often implies a human decision.

Note 2: Determination is a superordinate concept of *measurement* and examination [16] and so the term "determination" should not be used when "measurement" applies.

Note 3: ISO 9000 defines determination as "activity to find out one or more characteristics and their characteristic values" [32].

Source: [33]. See also *testing*.

2.29 interference

Process whereby a *measured quantity value* [VIM 2.10] is changed by an *influence quantity* [VIM 2.52].

Entry replaces recommendation in [34] p 554.

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2.30 interferent

Component of the *matrix* that embodies an *influence quantity* [VIM 2.52].

Example: In the analysis of arsenic using inductively coupled plasma-mass spectrometry at low mass resolution the presence of chloride in the *analytical sample* causes the formation of $^{40}Ar^{35}Cl^{+}$ which has the same *m*/*z* value of 75 as As^{+}.

2.31 intermediate measurement precision
intermediate precision

Measurement precision [VIM 2.15] under *intermediate precision conditions of measurement* [VIM 2.22].

Source: [VIM 2.23].

Note: "Intralaboratory precision" or "within-laboratory precision" is sometimes used as a synonym of intermediate measurement precision.

2.32 internal standard

Component used for reference present in or added to a *sample* to perform *calibration* [VIM 2.39] or to assist in identification of a chemical species, or as part of *procedure validation*.

Note 1: An internal standard provides an *indication* [VIM 4.1] that varies in the same way as that of the *analyte* during *chemical analysis*. The ratio of the indications for analyte and internal standard provides a *quantity value* [VIM 1.19] that can be used in calibration.

Note 2: In multicomponent mixtures, a component that is known to be in constant concentration or content across samples can be used as an internal standard.

Note 3: An added internal standard may be a *spike*.

Entry replaces recommendation in [35] p 837.

2.33 laboratory bias

Contribution to *measurement bias* [VIM 2.18] that is attributed to *systematic effects* on *measurement results* [VIM 2.9] made in a laboratory.

Note: Measurement bias in *analytical chemistry* may be considered to include *run bias*, laboratory bias, and *measurement procedure bias.*

2.34 laboratory sample

Sample as prepared for sending to a laboratory and intended for *inspection* or *testing*.

Note: When no preparation of a laboratory sample is required, the laboratory sample is an *analytical sample*.

Source: [16] Appendix B. See also *primary sample*, *aliquot*.

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2.35 limit of detection, (LOD)
detection limit, (DL)

True quantity value [VIM 2.11] for a *quantity* [VIM 1.1] of a *component* present in a material for which the probability of falsely claiming the absence of the component is β, given a probability α of falsely claiming its presence based on an established criterion for detection.

Note 1: The limit of detection is usually considered to be a *performance characteristic of a measurement procedure*, performed in a particular laboratory.

Note 2: The quantity is usually a mass fraction or a concentration but can also be for example, a mass or an amount of substance.

Note 3: The established criterion for detection can be, for example, a *critical value* which leads to a declaration that the component is present.

Note 4: IUPAC recommends default values for α and β equal to 0.05. This corresponds to requiring a level of confidence (see *coverage probability* [VIM 2.37] Note 2) of 95 % for a statistical test for non-zero true value of the quantity, and to a statistical power of 95 % for that test applied to a material containing the component at the limit of detection.

Note 5: The limit of detection is not a criterion for detection but indicates the true value of a quantity of the component in a material that can be detected reliably, given a separate criterion (for example critical value) for declaring the component present.

Note 6: If the limit of detection is estimated as a multiple of the standard deviation of *measured quantity values* [VIM 2.10] of a *blank material* (or one spiked with a small *aliquot* of the component) measured under *repeatability conditions of measurement* it is important to document the multiplication factor applied so that different values stated for limits of detection can be compared.

Note 7: The letter symbols LOD and DL should not replace the quantity symbol but may be given as subscript to the appropriate symbol for the quantity, e.g. w_{LOD}, m_{DL}.

Note 8: In ISO 3534-2, ‘minimum detectable value of the net state variable’ is defined as “true value of the net state variable in the actual state that will lead, with probability, 1 − error probability, to the conclusion that the system is not in the basic state.” [4]

Note 9: According to the definition given here and in ISO 11843, LOD is a (unobservable) true value. This differs from the definition in VIM 4.18 where the concept ‘detection limit’ refers to a measured quantity value. [1]

Note 10: In some European legislation ‘detection capability’ (denoted $CC\beta$) is defined as “the smallest content of the substance that may be detected, identified and/or quantified in a sample with an error probability of β”. [30]

Note 11: The ISO 11843 series “Capability of detection” covers a wide field relating to “the detection of a difference between an actual state of a system and its basic state”, which additionally includes cases in which the "basic state" does not correspond to absence (zero concentration) of a component. [36]

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Note 12: The use of the term "sensitivity" for limit of detection is erroneous as it refers to the slope of the *calibration curve*.

Note 13: The US Environmental Protection Agency defines 'method detection limit' (MDL) as "the minimum measured concentration of a substance that can be reported with 99 % confidence that the measured concentration is distinguishable from method blank results". [37]

Sources: [8, 12, 31, 38]. Entry replaces recommendation in [8] p 5.

2.36 limit of quantification, (LOQ)
quantification limit

Smallest or largest *measured quantity value* [VIM 2.10], obtained by a given *measurement procedure*, which fulfils a *requirement* of *fitness for purpose*.

Note 1: The *quantity* [VIM 1.1] measured is usually a mass fraction or a concentration but can also be for example, a mass or amount of substance.

Note 2: The requirement can, for example, be a standard deviation under *repeatability conditions of measurement*, or a *measurement uncertainty* [VIM 2.26].

Note 3: The smallest and largest measured quantity value correspond to the lower limit of quantification (LLOQ) and the upper limit of quantification (ULOQ) respectively. The interval between LLOQ and ULOQ is the *working interval*.

Note 4: If the LLOQ is estimated as a multiple of the standard deviation of measured values of a *blank material* (or one spiked with a small *aliquot* of the *component*) obtained under repeatability conditions of measurement it is important to document the multiplication factor, which may be 5, 6 or 10, applied so that different values stated for LLOQ can be compared.

Reference: [31, 39].

2.37 linearity of a measuring system

Ability of a *measuring system* [VIM 3.2] to provide *measured quantity values* [VIM 2.10] that are directly proportional to the *quantity value* [VIM 1.19] of the *measurand*.

Source: [40]. See also [41].

Note 1: The linearity of a measuring system is assessed during *procedure validation.*

Note 2: The set of measured quantity values for which linearity of a measuring system applies is usually termed "linear interval" or "linear range".

Note 3: Linearity of a measuring system should not be confused with *linearity of calibration*.

2.38 linearity of calibration
calibration linearity

Closeness of agreement between *indications* [VIM 4.1] obtained using *calibrators* [VIM 5.12] in the first step of a *calibration* [VIM 2.39] and indications predicted by the *calibration function* for the calibrators' *reference values* [VIM 5.18].

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Note 1: The concept applies to calibration functions of any mathematical form. The term "linearity" is historical and refers to a time when calibration graphs were constructed on paper and were invariably considered to be linear.
Note 2: Linearity of calibration may be expressed by measures of agreement (e.g. correlation coefficient) or deviation (e.g. standard error of regression), obtained by regression of calibration data, or assessed from a residual plot ([5] entry 3.1.4). See also [42].
Note 3: Linearity of calibration is assessed during *procedure validation*.
Note 4: Calibration linearity should not be confused with *linearity of a measuring system*.
See also: [19].

2.39 lot

Material which is assumed to be uniform for the purpose of *sampling*.

Note: Some vocabularies assume "lot" and *"batch"* to be synonymous. The distinction made here with respect to knowledge of production history permits a lot to consist of one or more batches and is useful in interpreting the results of *chemical analysis*. See also definitions in ISO 11961 [43], ISO 472 [44], ISO 15736 [45], and ISO 18113-1 [46].
Source: Entry replaces recommendation in [17] entry 2.2.2.

2.40 mass balance

See: *chemical purity*.

2.41 material homogeneity
homogeneity

Uniform structure or composition of a material with respect to one or more specified properties.

Note 1: A material is said to be homogeneous with respect to a specified *quantity* [VIM 1.1] if the *quantity values* [VIM 1.19] measured using *aliquots* of specified size do not fall outside a specified interval. See *minimum sample size*.
Note 2: In the homogeneity study of a *candidate reference material* it is distinguished whether the *analytical samples* are taken from different supply units or from a single supply unit ("between-bottles homogeneity" or "within-bottle homogeneity", respectively).
Note 3: Inhomogeneity is a source of *measurement uncertainty* [VIM 2.26].
Note 4: Detailed guidance for the assessment of homogeneity of *reference materials* [VIM 5.13], is given in ISO Guide 35 [47].
Entry replaces recommendation in [17] p 1201.

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2.42 material recovery
recovery

Mass (volume, amount of substance) of a specified *component* isolated from a *system* divided by the mass (volume, amount of substance) of the system prior to isolation.

Source: [48].

Note 1: The *measurement unit* [VIM 1.9] of material recovery is the measurement unit of the *quantity* [VIM 1.1] related to the specified component divided by the unit of the quantity describing the system. When these units are the same material recovery may be expressed as a percentage, and the quantity specified.

Note 2: The term "recovery" is also used to describe a *recovered quantity value ratio*. Therefore, the term "recovery" should not be used without qualification unless the meaning is clear from the context.

See also: [49].

2.43 material stability
stability

Constancy of a property of a material over time.

Note 1: A material is said to be stable with respect to a specified property if its measured property values do not fall outside a specified interval during storage under specified conditions over a specified period of time.

Note 2: A *reference material* is assessed for the stability of an embodied property under conditions of transport ("short-term stability") and storage ("long-term stability").

Source: [2].

Note 3: The variation of the property value over time adds a contribution to the *uncertainty budget* [VIM 2.33] or the examination uncertainty [11], as applicable. Regarding the assessment of stability of reference material, detailed guidance is given in ISO Guide 35 [47].

Note 4: The term “stability” is also used for *stability of a measuring instrument* [VIM 4.19] or process (See: *control limit*).

2.44 matrix

Analytical sample excluding the *analyte*.

Note: In *matrix reference material* the concept ‘matrix’ is used in the sense of kind of material.

See also: *blank material* Note 2. Entry replaces recommendation in [18] p 1660.

2.45 matrix effect

Systematic measurement error [VIM 2.17] caused by the *matrix*.

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See also: *multiplicative matrix effect*, *additive matrix effect.* Entry replaces recommendation in [25] definition 1.

2.46 measurand

Quantity [VIM 1.1] intended to be measured.

Note 1: The *specification* of a measurand requires knowledge of the *kind of quantity* [VIM 1.2], description of the state of the phenomenon, body, or substance embodying the quantity, including any relevant *component*, and the chemical entities involved.

Note 3: The *measurement*, including the *measuring system* [VIM 3.2] and the conditions under which the measurement is carried out, might change the phenomenon, body, or substance such that the quantity being measured may differ from the measurand as defined. In this case, adequate *correction* [VIM 2.53] is necessary.

Example 2: The length of a steel rod in equilibrium with the ambient Celsius temperature of 23 °C will be different from the length at the specified temperature of 20 °C, which is the measurand. In this case, a correction is necessary.

Note 4: In chemistry, *analyte*, or the name of a substance or compound, are terms sometimes used for 'measurand'. This usage is erroneous because these terms do not refer to quantities.

Source: [VIM 2.3] with Note 2 and Example 1 omitted.

Example 3: The electric potential difference between the terminals of a battery may decrease when using a voltmeter with a significant internal conductance to perform the measurement. The open-circuit potential difference can be calculated from the internal resistances of the battery and the voltmeter.

Source: [VIM 2.3] Example 1 with minor clarification.

Note 5: The measurand may be operationally defined by reference to a documented *measurement procedure* to which only *quantity values* [VIM 1.19] obtained by the same procedure can be compared.

Source: [50].

Entry replaces recommendation in [51] p 980.

2.47 measurement

Process of experimentally obtaining one or more *quantity values* [VIM 1.19] that can reasonably be attributed to a *quantity* [VIM 1.1].

Note 1: Measurement does not apply to *nominal properties* [VIM 1.30].

Note 2: Measurement implies comparison of quantities or counting of entities.

Note 3: Measurement presupposes a description of the quantity commensurate with the intended use of a *measurement result* [VIM 2.9], a *measurement procedure*, and a calibrated *measuring system* [VIM 3.2] operating according to the specified measurement procedure, including the measurement conditions.

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Source: [VIM 2.1].

Note 4: Measurement is a subordinate concept of *determination* and so the term "determination" should not be used when "measurement" applies.

Note 5: If a measurement result is assessed with respect to conditions implied by a norm, standard, or *specification*, (i.e. in *conformity assessment*) measurement is often termed *testing*.

Entry replaces recommendation in [52] p 1565.

2.48 measurement procedure

Detailed description of a *measurement* according to one or more *measurement principles* [VIM 2.4] and to a given *measurement method* [VIM 2.5], based on a *measurement model* [VIM 2.48] and including any calculation to obtain a *measurement result* [VIM 2.9].

Note 1: A measurement procedure is usually documented in sufficient detail to enable an operator to perform a measurement.

Note 2: A measurement procedure can include a statement concerning a *target measurement uncertainty*.

Source: [VIM 2.6] with Note 3 omitted.

Note 4: Measurement procedures in chemistry can be structured according to ISO 78-2 [53] or Annex A of the Eurachem Guide [19].

Note 5: An authorised measurement procedure is sometimes termed "*standard operating procedure*" (SOP), or "recommended operating procedure" (ROP).

Note 6: In ISO/IEC 17025 [22] the term "method" is used for measurement procedure. "Examination procedure" is defined for medical laboratories [6, 54].

Note 7: The historical term "assay" is now largely obsolete as a synonym for metrological terms such as measurement procedure, but still used in composite terms e.g. *immunoassay*, *bioassay*.

2.49 measurement procedure bias

measurement method bias

Contribution to *measurement bias* [VIM 2.18] that is attributed to *systematic effects* on *measurement results* [VIM 2.9] made according to a *measurement procedure*.

Note 1: Measurement procedure bias covers *instrumental bias* [VIM 4.20].

Note 2: Contributions to measurement procedure bias are calculated during *procedure validation* [19].

Note 3: Measurement bias in *analytical chemistry* may be considered to include *run bias*, *laboratory bias*, and measurement procedure bias [55].

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2.50 measurement procedure with standard addition
standard addition

Measurement procedure in which *indications* [VIM 4.1] are obtained for an *analytical sample* as well as for analytical samples with addition(s) of a *measurement standard* [VIM 5.1].

Note 1: A measurement procedure with standard addition provides an unbiased *measurement result* [VIM 2.9] if there is a *multiplicative matrix effect*.

Source: [13].

2.51 measurement reproducibility
reproducibility

Measurement precision [VIM 2.15] under *reproducibility conditions of measurement* [VIM 2.24].

Note 1: Relevant statistical terms are given in ISO 5725-1:1994 [56] and ISO 5725-2:2019 [57].

Source: [VIM 2.25].

Note 2: The term “interlaboratory precision” or “between-laboratory precision” is sometimes used as a synonym of measurement reproducibility.

2.52 measuring interval

See: *working interval*.

2.53 metrological compatibility of measurement results
metrological compatibility

Property of a set of *measurement results* [VIM 2.9] for a specified *measurand*, such that the absolute value of the difference of any pair of *measured quantity values* [VIM 2.10] from two different measurement results is smaller than some chosen multiple of the *standard measurement uncertainty* [VIM 2.30] of that difference.

Note 1: Metrological compatibility of measurement results replaces the traditional concept of ‘staying within the error’, as it represents the criterion for deciding whether two measurement results refer to the same measurand or not. If in a set of *measurements* of a measurand, thought to be constant, a measurement result is not compatible with the others, either the measurement was not correct (e.g. its *measurement uncertainty* [VIM 2.26] was assessed as being too small) or the measured *quantity* [VIM 1.1] changed between measurements.

Note 2: Correlation between the measurements influences metrological compatibility of measurement results. If the measurements are completely uncorrelated, the standard measurement uncertainty of their difference is equal to the root mean square sum of their standard measurement uncertainties, while it is lower for positive covariance or higher for negative covariance.

Source: [VIM 2.47].

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Note 3: As required by the Mutual Recognition Arrangement (MRA) of the International Committee for Weights and Measures (CIPM) through which national metrology institutes demonstrate the international equivalence of their *measurement standards* [VIM 5.1], the concept 'degree of equivalence' is applied in special *interlaboratory comparisons* termed "key comparisons". The degree of equivalence of each *national measurement standard* [VIM 5.3] is expressed quantitatively by two terms: its deviation from the *reference value* [VIM 5.18] of the key comparison and the measurement uncertainty of this deviation (at a level of confidence of approximately 95 %). See also *metrological equivalence of measurement results*.

Source: [58].

2.54 metrological equivalence of measurement results
equivalence of measurement results

Property of two or more *measurement results* [VIM 2.9] for a given *measurand* that have *metrological compatibility of measurement results*, so that they are each acceptable for the same specified intended use.

Note: Measurement results are either metrologically equivalent or they are not.

Source: [59].

2.55 minimum sample size
minimum sample intake

Lower limit of sample size stipulated in documentation taken for *chemical analysis*.

Note 1: Examples of documentation include a *measurement procedure*, product information sheets (see *reference material*) and *reference material certificates*.

Note 2: Values associated with *performance characteristics of a measurement procedure* and the property values stated in documentation are rendered invalid if the minimum sample size is not taken.

Source: Adapted from [2] entry 2.1.8.

2.56 multiplicative matrix effect

Matrix effect that is proportional to the *measured quantity value* [VIM 2.10] of the *measurand*.

Note 1: A multiplicative matrix effect can be compensated for by following a *measurement procedure with standard addition*.

Note 2: A multiplicative matrix effect affects the slope, not the intercept of a linear *calibration curve*.

Note 3: The effect is sometimes termed "rotational matrix effect" or "proportional interference" [13].

Note 4: A multiplicative matrix effect may originate from non-analyte *components* of the *measurement standard* [VIM 5.1] if these contribute to the signal attributed to the *analyte*.

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2.57 non-certified property value

Property value that is provided for information only but is not certified by a *reference material producer*.

Note 1: A non-certified property value cannot be used as reference in a *metrological traceability chain* [VIM 2.42].

Note 2: A non-certified property value may be included in the *reference material certificate* or supplied in other form.

Note 3: In ISO Guide 30 [2] "indicative value", "information value", and "informative value" are admitted terms.

Source: [2, 60].

2.58 object traceability
traceability
deprecated: trackability

Ability to trace the history, application or location of an object.

Note 1: When considering a product or a service, traceability can relate to: the origin of materials and parts; the processing history; or the distribution and location of the product or service after delivery.

Note 2: In [61] the term defined is traceability. However, because of the potential confusion with *metrological traceability* [VIM 2.41] it is recommended to use the full term if there is ambiguity.

Source: [61].

2.59 primary sample

Collection of one or more *sampling increments* initially taken from material intended to be analysed. Source: [17].

Note 1: The term primary, in this case, does not refer to the *quality* of the *sample*, rather the fact that the sample was taken during the earliest stage of *measurement*.

See also [16] Appendix B.

2.60 property value assignment
value assignment

Determination of property values obtained in the course of the production of a *reference material*.

Source: [2]. See also *assigned value*

2.61 recovered quantity value ratio
analytical recovery
recovery

Measured quantity value [VIM 2.10] relating a *component* to a *system* divided by a *reference value* [VIM 5.18].

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Note 1: The *quantities* [VIM 1.1] involved are rational *unitary quantities* and of the same *kind of quantity* [VIM 1.2], usually either a concentration or content.

Note 2: The respective *measurement procedure* must be specified.

Note 3: The definition can be symbolized by $R_B = \frac{Q_{B,measured}}{Q_{B,ref}}$, where R denotes the recovered ratio of the *quantity values* [VIM 1.19] Q and B identifies the component.

Note 4: The term "recovery" is also used to describe *material recovery*. Therefore, the term "recovery" should not be used without qualification unless the meaning is clear from the context.

Note 5: Recovery quantity value ratio is used in *procedure validation* to evaluate and correct for the *measurement procedure bias*. [19]

Note 6: Recovered quantity value ratio may be estimated from the measured change of the quantity value of the component of interest upon addition of a known amount of substance or mass of the component. The added material containing the component is often termed *spike*. See also *blank material* Note 5, *measurement procedure with standard addition, spike*.

Source: [19, 49]. Entry replaces recommendation in [25] definition 2.

2.62 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* [VIM 3.2], same operating conditions and same location, and replicate measurements on the same or similar objects over a short period of time.

Note 1: A condition of measurement is a repeatability condition only with respect to a specified set of repeatability conditions.

Source: [VIM 2.20] with Note 2 omitted.

Note 3: In ISO 3534-2 "same operator" (singular) is stipulated as a repeatability condition. The VIM request of "same operators" (plural) should be understood that if two or more operators contribute to one measurement, they should be involved in the same way in repeated measurements [4].

Note 4: In *analytical chemistry* the phrase "under repeatability conditions" refers to the above specified set of conditions.

Note 5: A set of measurements under repeatability conditions is often termed *analytical run*.

2.63 replicate (duplicate) samples

Multiple (two) *samples* taken under compatible conditions.

Note 1: This selection may be accomplished by taking *sampling increments* 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.

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Source: [17] p 1203.

Note 2: In ISO 3534-2:2006 "replicate sampling" is defined [4] entry 5.2.5.

2.64 run bias

Contribution to *measurement bias* [VIM 2.18] that is attributed to *systematic effects* on *measurement results* [VIM 2.9] made in a single *analytical run*.

Note: Measurement bias in *analytical chemistry* may be considered to include run bias, *laboratory bias*, and *measurement procedure bias*.

2.65 sample

Portion of a material taken for *qualitative analysis* or *quantitative analysis*.

Note 1: Taking a sample from a material implies the existence of a sampling error [16], i.e. the *measured quantity values* [VIM 2.10] of the portion's properties are only estimates of those of the parent material.

Note 2: If the portion is removed with negligible sampling error it is termed an *aliquot*, or specimen. "Specimen" is used to denote a portion taken under conditions such that the sampling variability cannot be assessed, and is assumed, for convenience, to be zero.

Note 3: The *sampling plan* should detail how a sample is obtained and any subsequent manipulations (See: *sample pre-treatment*).

Note 4: Fundamentals of sampling and sample pre-treatment in *analytical chemistry* are detailed in [62, 63].

Note 5: In analytical chemistry 'sample' must not be confused with a subset of a population for which the term "sample" is used in statistics.

Source: [8]. See also: *analytical sample*, *primary sample*, *replicate sample*, *spike*. Entry replaces recommendation in [25] entry S05451 (https://doi.org/10.1351/goldbook.S05451).

2.66 sample pre-treatment
sample preparation

Collective noun for all procedures used for conditioning a *sample* to a defined state which allows subsequent examination [11] or *chemical analysis* or long-term storage (See: *material stability*).

Note: Sample pre-treatment includes e.g. mixing, splitting, drying, crushing, stabilization.

Source: [16] Appendix B.

2.67 sampling

Act of taking or constituting a *sample*.

Note: Sampling often provides a contribution to the *measurement uncertainty budget* [VIM 2.33] or the examination uncertainty [11], as applicable. See: [16].

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Source: [4].

2.68 sampling increment
increment

Individual portion of material collected by a single operation of a sampling device.

Source: [16] Appendix B. See also *primary sample.*

2.69 sampling target

Portion of material, at a particular time, that the *sample* is intended to represent.

Note 1: The sampling target should be defined prior to designing the *sampling plan*.
Note 2: The sampling target may be defined by Regulations (e.g. *lot* size).

Source: [16] Appendix B.

2.70 sampling plan

Predetermined procedure for the selection, withdrawal, preservation, transportation and preparation of the portions to be removed from a material as a *sample*.

Source: [16] Appendix B. Entry replaces recommendation in [17] p 1201.

2.71 shelf life

Time interval during which a *reference material producer* warrants the *material stability* of the *reference material*.

Note: The shelf life is equivalent to the "period of validity" of the *reference material certificate* and is ended by the “expiry date”.

Source: [47].

2.72 spike

Material with known *quantity values* [VIM 1.19] added to an *analytical sample*.

Note 1: The material can be a *reference material* or a *certified reference material* [VIM 5.14].
Note 2: The known quantity value is often a fraction or concentration.
Note 3: A spike may be used to estimate *recovered quantity value ratio* or compensate for *systematic measurement error* [VIM 2.17].
Note 4: “Spike” used as a verb is the addition of a spike to a *sample*.

2.73 system

Part or phenomenon of the perceivable or conceivable universe consisting of a demarcated arrangement of a set of entities and a set of relations between these entities.

Source: [26].

Note 1: In *analytical chemistry* "system" often denotes a material.

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Example 1: The tailings dam of a mine containing water and suspended solids, heavy metals and other *chemical substances*, at a particular time, subject to investigation by an environmental protection agency.

Example 2: Residue from a flask suspected to contain illegal drugs seized by the police and submitted for forensic examination.

Note 2: The VIM defines *measuring system* [VIM 3.2] as "a set of one or more *measuring instruments* [VIM 3.1]".

2.74 systematic effect

Recognized effect of an *influence quantity* [VIM 2.52] on a *measured quantity value* [VIM 2.10].

Note: A systematic effect can be compensated for by a *correction* [VIM 2.53].

2.75 testing
test

Determination of one or more characteristics of an object of *conformity assessment*, according to a specified procedure.

Source: [64]. See also: *inspection*.

Note: In *analytical chemistry* testing may be *measurement* to obtain a *quantity value* [VIM 1.19] or an examination [11] such as identifying a *chemical substance* (see *qualitative analysis*).

2.76 unitary quantity

Quantity [VIM 1.1] with a magnitude expressed as a reference quantity multiplied by a number.

Note: The concept is denoted in the VIM as "quantity expressed by a *measurement unit* [VIM1.9]" and referred to in Note 1 to [VIM 2.41]as "non-ordinal quantity". See Figure A.1 of [1].

Source: [65]. See also: [26].

2.77 working interval
working range

Set of *quantity values* [VIM 1.19] over which a *measuring instrument* [VIM 3.1] or *measuring system* [VIM 3.2] provides *measurement results* [VIM 2.9] with acceptable *measurement uncertainty* [VIM 2.26], under defined conditions.

Note 1: In some fields, the term is "measuring interval" [VIM 4.7] or "measurement range".

Note 2: The working interval is bounded by the lower and upper *limit of quantification*.

Note 3: The lower limit of a working interval should not be confused with *detection limit*.

Source: [19] section 6.3.

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3 QUALITY AND QUALITY MANAGEMENT

The Recommendations in this section will contribute to the final chapter in the 4th edition of the Orange Book (Compendium of Terminology in Analytical Chemistry). It contains a vocabulary of concepts, partly related to quality in general, and partly to the specific measures that a laboratory undertakes to demonstrate fitness for purpose of its results [66]. These specific concepts build on the fundamental terminology of the International Vocabulary of Metrology, 3rd edition [1]. In chemistry Eurachem, CITAC, ILAC and other bodies have contributed to our understanding of *quality* as it relates to chemical measurement results.

In analytical laboratories quality assurance [21, 67] is the essential organisational infrastructure that underlies all quality matters such as staff training and management, adequacy of the environment, safety, the storage, integrity and identity of samples, record keeping, the maintenance and calibration of instruments, and the use of technically validated and properly documented measurement procedures. Failure in any of these areas might undermine vigorous efforts elsewhere to achieve the desired quality of data. In recent years these practices have been codified and formally recognised as essential. However, the prevalence of these favourable circumstances by no means ensures the attainment of appropriate data quality unless quality control is conducted [21].

Faced with a customer request, the laboratory translates this into an analytical requirement, i.e. what performance is required by the method. The laboratory may develop and validate a new analytical procedure or verify that an existing one meets the requirements. Subsequent routine application of the procedure is supported by internal and external technical and administrative measures, such as statistical process control, participation in interlaboratory comparisons and audits. All these measures should verify that the laboratory continues to provide fit-for-purpose results, which enables the customer or another end-user to make technically and administratively correct decisions.

Various terms are used to describe the core technical work of a laboratory or related activities. While measurement, so far, has been restricted to a quantitative aspect, others, e.g. “analysis”, “testing”, “examination”, “inspection” and “determination” are generally used in a broader sense, i.e. to cover also a qualitative aspect. In addition, these terms are part of other terms indicating the organization where the work is performed, e.g. “testing laboratory”, and “inspection body”.

Customers and/or statutory and regulatory bodies may require the laboratory to demonstrate conformance (compliance) with written national or international standards, and to demonstrate its technical competence for the services it provides. Laboratories, therefore, often implement a quality management system and subsequently apply for accreditation. This is a strategic decision for the laboratory that can help improving its overall performance and provide a sound basis for sustainable development initiatives.

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3.78 acceptance interval
acceptance zone

Interval of permissible *measured quantity values* [VIM 2.10].

Note 1: Permissible measured quantity values are associated with objects that conform to a *specification*. (See Note 2 of *conformity assessment*).
Note 2: Unless otherwise stated in the specification, the *acceptance limits* belong to the acceptance interval.
Note 3: An acceptance interval is termed an "acceptance zone" in the Eurachem guide on compliance assessment [68].

Source: [69]. See also *rejection interval*.

3.79 acceptance limit

Specified upper or lower bound of permissible *measured quantity values* [VIM 2.10].

Note: Permissible measured values are associated with items that conform to a *specification* and lie within the *acceptance interval* for the item.

Source: [69]. See also *conformity assessment*.

3.80 accreditation of a laboratory

Third-party attestation related to a laboratory conveying formal demonstration of its *competence* to carry out specific *conformity assessment* tasks.

Example: Accreditation of an *analytical chemistry* laboratory to ISO/IEC 17025 [22] for the *measurement* of the mass concentration of lead in environmental *samples*.
Note 1: Examples of conformity assessment tasks for which accreditation can be granted are measurement, *testing*, *inspection*, provision of *proficiency testing schemes* and production of *reference materials*.
Note 2: The criteria for determining a laboratory's competence are based on relevant international standards, e.g. ISO/IEC 17025 [22], ISO 15189 [54], or ISO 15195 [70] and include adequate *quality assurance* and *quality control* procedures, such as qualifications, training and experience of staff, appropriate equipment that is properly calibrated and maintained, use of validated *measurement procedures*, participation in *interlaboratory comparisons*, and appropriate sampling practices.

Source: [64].

3.81 analytical selectivity
selectivity

Extent to which an analytical *measurement procedure* can be used to determine a property of a particular *component* in a material without *interferences* from other components having similar behaviour.

Note: Selectivity should be qualified by "analytical" if there is potential confusion with selectivity in catalysis, or in organic reaction mechanisms.

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Source: [71]. See also [19], *selectivity of a measuring system* [VIM 4.13]. Entry replaces recommendation in [34] p 555.

3.82 assessor

Person with relevant professional expertise and experience who can evaluate the *competence* of a laboratory on behalf of an accreditation body.

Note 1: The person may be engaged in a voluntary or paid capacity.
Note 2: The work of an assessor can be termed “peer review”.
Note 3: Depending on the role and responsibilities of an assessor, terms such as "lead assessor" and "technical assessor" are often used.

3.83 assigned value

Value attributed to a particular property of a *test* item and that serves as an agreed reference for comparison.

Note 1: The value may be a *reference quantity value* [VIM 5.18] or a value of a *nominal property* [VIM 1.30].
Note 2: Options for establishing an assigned value for some types of *proficiency testing schemes* are detailed in ISO/IEC 17043 [29] and ISO 13528 [27].

Sources: [29], [72] entry 2.7. See also *property value assignment.*

3.84 audit

Systematic, independent and documented process for obtaining objective evidence and evaluating it objectively to determine the extent to which the audit criteria are fulfilled.

Note 1: The fundamental elements of an audit include the *determination* of the conformity of an object according to a procedure carried out by personnel not being responsible for the object audited.
Note 2: An audit can be an internal audit (first party), or an external audit (second party or third party), and it can be a combined audit or a joint audit.
Note 3: Internal audits, sometimes termed first-party audits, are conducted by, or on behalf of, the *organization* itself for management review and other internal purposes, and can form the basis for an organization’s declaration of conformity. Independence can be demonstrated by the freedom from responsibility for the activity being audited.
Note 4: External audits include those generally termed second and third-party audits. Second-party audits are conducted by parties having an interest in the organization, such as customers, or by other persons on their behalf. Third-party audits are conducted by external, independent auditing organizations such as those providing *certification*/registration of conformity or governmental agencies.

Source: [61] entry 3.13.1.

3.85 candidate certified reference material
candidate CRM

Reference material subjected to a process of *reference material certification.*

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3.86 candidate reference material
candidate RM

Material subjected to the procedures necessary to show its fitness for intended use (See: *fitness for purpose*).

Note: A candidate reference material for a given property may already be a *reference material* for other properties.

Source: [2].

3.87 capability

Ability of an object to realize an output that will fulfil the *requirements* for that output.

Note: Process capability terms in the field of statistics are defined in ISO 3534-2 [4].

Source: [61].

3.88 cause-and-effect diagram
Ishikawa diagram
herringbone diagram
fishbone diagram

Diagram indicating the causes of a specific event or condition.

Note: In *analytical chemistry*, Ishikawa diagrams are used to indicate sources of *measurement uncertainty* [VIM 2.26]. See Figure 3.88-1.

Source: [73].

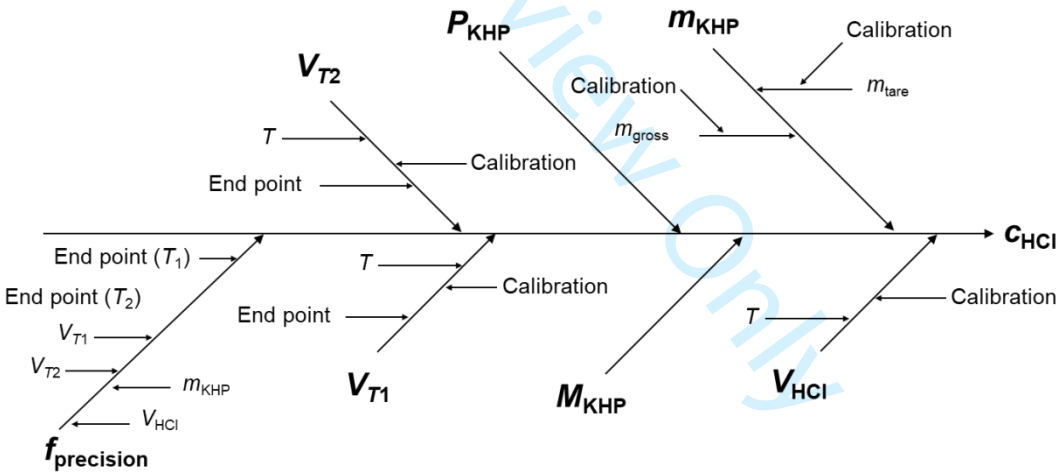

Figure 3.88-1. Ishikawa diagram for the titration of a hydrochloric acid solution with sodium hydroxide solution that has been standardized using potassium hydrogen phthalate (KHP). When used for identification of sources of *measurement uncertainty*, the diagram illustrates how the *quantity value* [VIM 1.19] of the *measurand* (c_{HCl}) depends on *input quantities in a measurement model* [VIM 2.50] (symbols in bold) which in turn depend on other *quantities* [VIM 1.1]. Symbols have their usual meanings. $f_{precision}$ is a is a factor in the *measurement function* [VIM 2.49] to account for

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measurement precision [VIM 2.15] with value 1 and *standard measurement uncertainty* [VIM 2.30] (See [73] Fig. A3.5).

3.89 certification

Third-party attestation related to products, processes, systems or persons.

Note 1: Certification of a management system is sometimes also termed registration.
Note 2: Certification is applicable to all objects of *conformity assessment* except for conformity assessment bodies themselves, to which accreditation is applicable.

Source: [64].

3.90 commutability of a reference material

Property of a *reference material*, demonstrated by the closeness of agreement between the relation among the *measurement results* [VIM 2.9] for a stated *quantity* [VIM 1.1] in this material, obtained according to two given *measurement procedures*, and the relation obtained among the measurement results for other specified materials.

Note 1: The reference material in question is usually a *calibrator* and the other specified materials are usually routine *samples*.
Note 2: The measurement procedures referred to in the definition are the one preceding and the one following the reference material (calibrator) in question in a *calibration hierarchy* [VIM 2.40] (see ISO 17511 [74]).
Note 3: The *material stability* of commutable reference materials should be monitored regularly.

Source: [VIM 5.15].

Note 4: Cases in which a *reference material producer* is required to conduct assessment of commutability are outlined in ISO 15194 [75].
Note 5: Guidance for assessment of commutability of reference material in laboratory medicine is provided by IFCC [76-78].

3.91 competence

Ability to apply knowledge and skills to achieve intended results.

Note: Demonstrated competence is sometimes referred to as “qualification”.

Source: [61].

3.92 conformance probability

Probability that an item fulfils a specified *requirement*.

Source: [69].

3.93 conformity assessment
compliance assessment

Demonstration that specified *requirements* relating to a product, process, system, person or body are fulfilled.

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Note 1: The subject field of conformity assessment includes activities, such as *testing*, *calibration* [VIM 2.39], carrying out an *audit*, *inspection* and *certification*, as well as the accreditation of conformity assessment bodies.

Note 2: The expression "object of conformity assessment" or "object" is used to encompass any particular material, product, installation, process, system, person or body to which conformity assessment is applied.

Source: [64].

Note 3: "Body" refers to an *organization*.

See also *tolerance interval*, *acceptance interval*, *rejection interval*, *decision rule, guard band* and Figures 3.102-1 and 3.102-2.

3.94 control chart

Chart with *control limits* on which some statistical measure related to a series of *samples* is plotted in a particular order to steer the process with respect to that measure.

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

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

Source: [4].

Note 3: Examples of control charts are *Shewhart means chart*, *Shewhart range chart* and *cumulative sum control chart*.

Note 4: Control charts are commonly used in the regular monitoring of the performance of a *measurement procedure*, as part of the laboratory's *internal quality control*.

3.95 control limit

Value defining an intended level of stability for a process.

Source: [79].

Note 1: A control limit may be a statistical value or be related to a predetermined target value, calculated e.g. from a *target measurement uncertainty*. See [80].

Note 2: A typical *control chart* will consist of a centre line that reflects the level around which the plotted statistic can be expected to vary. In addition, this control chart will have two lines, called control limits, placed one on each side of the centre line that define a band within which the statistic can be expected to lie randomly if the process is in control.

Note 3: Control limits on a *Shewhart chart* are placed at a distance of $\pm 2\sigma$ and $\pm 3\sigma$ where σ is the known or estimated standard deviation of the population [81]. This gives approximate probabilities of 0.05 and 0.003 respectively of finding values outside the control limits. These limits are known as upper and lower warning limit (UWL, LWL) and upper and lower action limit (UAL, LAL) respectively. See Figure 3.159-1.

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Note 4: A typical response to a value outside a warning limit is to monitor the process and, if this condition is repeated, to stop and investigate.

Note 5: A value outside an action limit is normally taken as evidence that the process is no longer in statistical control. A typical response to such a value is to stop and investigate. (See: *process in a state of statistical control*).

3.96 coordinator of an interlaboratory comparison
coordinator

Person(s) with responsibility for organizing and managing all of the activities involved in the operation of an *interlaboratory comparison*.

Source: [29].

3.97 cumulative sum control chart, (CUSUM chart)

Control chart where the cumulative sum of deviations of successive *measured quantity values* [VIM 2.10] from a *reference value* [VIM 5.18] is plotted to detect shifts in the level of the *measurand*.

Note 1: The ordinate of each plotted point represents the algebraic sum of the previous ordinate and the most recent deviation from the reference, target, or control value.

Note 2: The best discrimination of changes in level is achieved when the reference value is equal to the overall mean value.

Note 3: The chart can be used for control, diagnostic, or predictive purposes.

Note 4: When used for process control, it can be interpreted graphically by a mask (e.g. V-mask) superimposed on the graph. An *out-of-control criterion* is when the path of the cumulative sum intersects or touches the boundary of the mask.

Source: [4].

Note 5: More suited to spreadsheet analysis, the following *quantities* [VIM 1.1] are calculated for N measured quantity values x_i ($i = 1 \ldots N$)
$S_{\mathrm{hi}}(i) = \max(0, S_{\mathrm{hi}}(i-1) + x_i - \mu - k)$; $S_{\mathrm{hi}}(0) = 0$
$S_{\mathrm{lo}}(i) = \max(0, S_{\mathrm{lo}}(i-1) - x_i + \mu - k)$; $S_{\mathrm{lo}}(0) = 0$
μ is a suitably chosen target value, and k is a reference value such that only shifts away from the target value greater than k will add to the cumulative sum. k is usually taken as half the shift in the process mean that is required to be detected divided by the standard deviation (σ) obtained under *repeatability conditions of measurement*. An *out-of-control criterion* is when $S_{\mathrm{hi}}(i)$ or $S_{\mathrm{lo}}(i)$ becomes greater than a limiting value h (usually $h = 4\sigma$). (Note that the reference value k is not a *coverage factor* [VIM 2.38]).

Note 6: CUSUM charts are particularly sensitive to reveal small *measurement bias* [VIM 2.18].

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3.98 decision rule in conformity assessment
decision rule

Documented rule that describes how *measurement uncertainty* [VIM 2.26] will be accounted for with regard to accepting or rejecting an item, given a specified *requirement* and a *measured quantity value* [VIM 2.10].

Source: [69]. See also *conformity assessment*.

Note: Decision rules in conformity assessment give a prescription for the acceptance or rejection of an item based on the measured quantity value, the associated measurement uncertainty and limit(s) expressed or implied by *specification*, taking into account the acceptable level of the probability of making a wrong decision. On the basis of the decision rules, an "*acceptance interval*" and "*rejection interval*(s)" are determined, such that if the measured quantity value lies in the acceptance interval the item is declared as conforming and if in the rejection interval it is declared as non-conforming. See [68].

3.99 fitness for purpose
fitness for intended use

Ability of a product, process or service to serve a defined purpose under specific conditions.

Source: [66].

3.100 good laboratory practice, (GLP)

Quality system concerned with the organisational process and conditions under which non-clinical health and environmental safety studies are planned, performed, monitored, recorded, archived, and reported.

Note 1: GLP is generally associated with the guidelines laid down by the Organization for Economic Co-operation and Development (OECD). The use of the term GLP outside these guidelines is not recommended.

Note 2: A GLP approval should not be confused with *accreditation of a laboratory*.

Source: [82].

3.101 good manufacturing practice, (GMP)

Combination of manufacturing and quality procedures aimed at ensuring that products are consistently manufactured to their specifications, and to avoid contamination of the product by internal or external sources.

Source: [83]. See also: [84].

3.102 guard band

Interval between a *tolerance limit* and a corresponding *acceptance limit*.

Note 1: The guard band includes the limits.

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Note 2: If the acceptance limits lie within the tolerance limits the decision for conformity of the item is known as guarded acceptance. The probability of falsely accepting a non-conforming item is reduced. This is most often found in chemistry. See Figure 3.102-1.

Note 3: If the acceptance limits lie outside the tolerance limits the decision for conformity of the item is known as guarded rejection. The probability of falsely rejecting a conforming item is reduced. See Figure 3.102-2.

Source: [69] entry 3.3.11. See also *conformity assessment*.

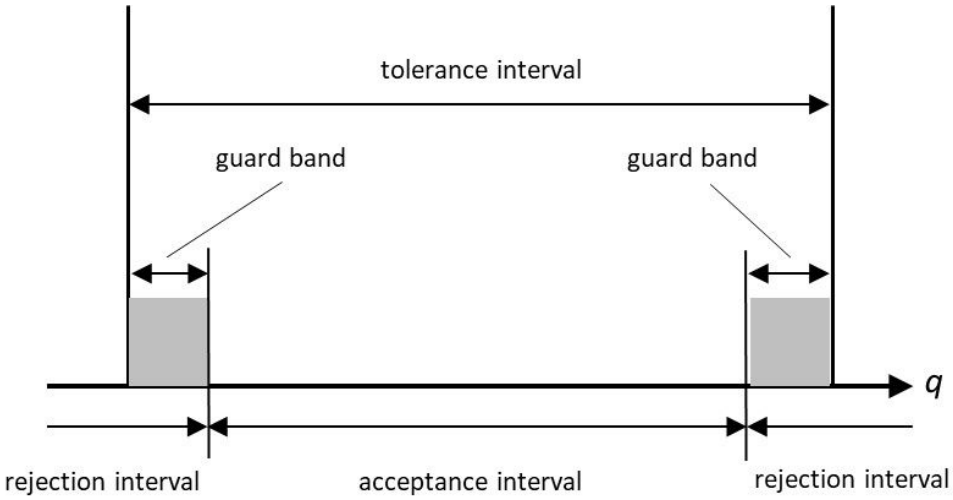

Figure 3.102-1: Guarded acceptance. Two-sided *acceptance interval* created by reducing the *tolerance interval* of permissible *measured quantity values* on either side by a guard band, thus reducing the probability of falsely accepting a non-conforming item.

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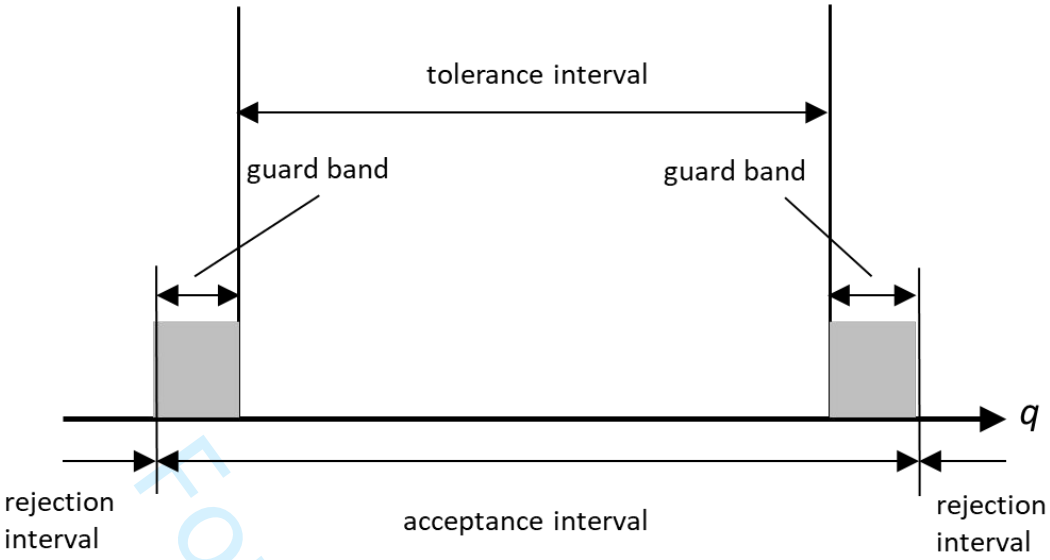

Figure 3.102-2: Guarded rejection. Two-sided acceptance interval created by increasing the tolerance interval of permissible *measured quantity values* on either side by a guard band, thus reducing the probability of falsely rejecting a non-conforming item.

3.103 Horwitz equation

Horwitz trumpet curve
Horwitz horn curve
Horwitz curve

Empirical relationship providing a standard deviation under *reproducibility conditions of measurement* [VIM 2.24] ($s_{R,H}$) to be expected for typical *measurements* of the mass fraction (w) of a *component* in a material: $s_{R,H} = 0.02w^{0.8495}$.

Note: The shape of the curve is called a trumpet [85] when the relative standard deviation is plotted against the logarithm of the mass fraction as shown in Figure 3.103-1. The reference justifies the mirror curve for negative ordinate values by: "… the lines are best regarded as confidence boundaries."

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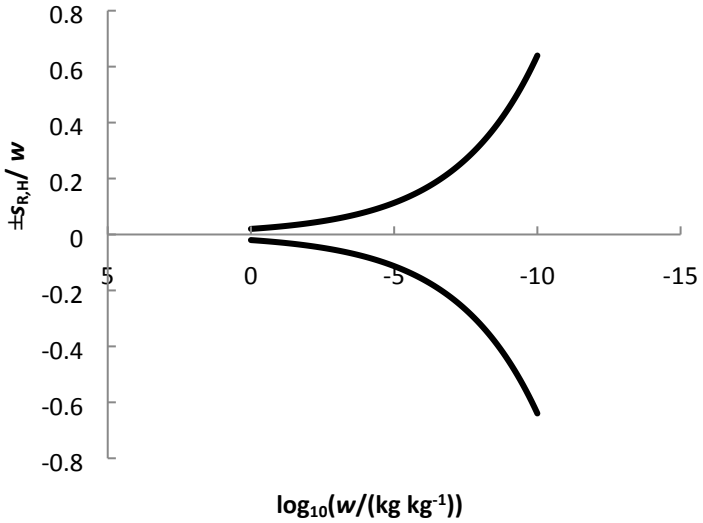

Figure 3.103-1: Horwitz curve (trumpet, horn). Expected relative standard deviation under reproducibility conditions of measurement, $\pm s_{R,H}/w$ plotted against logarithm of mass fraction, w.

Source: [85].

3.104 Horwitz ratio, (Horrat, HorRat, HORRAT), H

Standard deviation of a mass fraction of a *component* under *reproducibility conditions of measurement* [VIM 2.24] divided by the corresponding standard deviation calculated from the *Horwitz equation*.

Note 1: The Horwitz ratio is used as a test of the *fitness for purpose* of methods of *chemical analysis*.

Note 2: The experimental measurement precision [VIM 2.15] is better than to be expected from the Horwitz equation if the Horwitz ratio is less than 1, and poorer if greater than 1. In practice, ratios between 0.5 and 2.0 are acceptable.

Note 3: In [86] the 'Horwitz ratio' is defined as the ratio of the standard deviation under reproducibility conditions of measurement and standard deviation under *repeatability conditions of measurement*. This use is discouraged because of the possibility of confusion with the older usage.

Source: [87].

3.105 in-house reference material
laboratory reference material

Reference material produced and used by an analytical laboratory.

Note 1: The preparation, characterization and use of in-house reference materials for quality control purposes, are described in ISO Guide 80 [88].

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Note 2: Various terms are used to distinguish among reference materials intended for different uses and with *assigned values* established applying different procedures.

See also: *conventional quantity value*, *property value assignment*.

3.106 inspection

Examination of a product, process, service, or installation or their design and *determination* of conformity with specific *requirements* or, on the basis of professional judgment, with general requirements.

Note 1: Inspection of processes can include personnel, facilities, technology or methodology.

Note 2: Inspection procedures or schemes can restrict inspection to examination only.

Note 3: If the result of an inspection shows conformity, it can be used for purposes of *verification*.

Note 4: The result of an inspection can show conformity or non-conformity or a degree of conformity, where conformity is defined as fulfilment of a requirement.

Source: [61, 89].

3.107 interlaboratory comparison, (ILC)

Organization, performance and evaluation of *measurements* or *tests* on the same or similar items by two or more laboratories in accordance with predetermined conditions.

Source: [29].

Note 1: Interlaboratory comparison is a generic term, the purpose and detailed objectives of an Interlaboratory comparison must be specified. Some types of Interlaboratory comparison have special names, e.g. *proficiency testing scheme* and key comparison [90].

Note 2: Interlaboratory comparisons are organized at all metrological levels and have the following steps in common. a) A *coordinator* plans the interlaboratory comparison; b) One or more items are sourced by the coordinator, assessed as appropriate, and distributed to the *participants in a interlaboratory comparison* with instructions; c) The participants conduct *measurements*, tests, examinations [11] or other work on the item(s) and report results back to the coordinator; d) The coordinator evaluates the results and provides feedback to the participants and; e) The coordinator and/or the participants act on the results.

Example 1: A *proficiency testing provider* may be requested by legislation to report an unsatisfactory result to a regulatory body (e.g. a false negative result for a test of an infectious disease).

Example 2: A coordinator of a *material characterisation study* for a *candidate reference material* may decide to ask for some measurements to be repeated.

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Example 3: A coordinator of an interlaboratory *method performance study* may decide to recommend the issuing of a *standard operating procedure*.

Note 3: In some circumstances, one of the laboratories involved in an interlaboratory comparison may be the laboratory that provides the *assigned value* for the item. The operation enables the *determination* of the *metrological equivalence of measurement results* of the participants but does not, by itself, establish *metrological traceability* [VIM 2.41].

Note 4: The minimum number of laboratories participating in an interlaboratory comparison will depend on the metrological properties of the *measurement procedures* used. See [47, 91].

Note 5: Determination of *performance characteristics of a measurement procedure* as part of *procedure validation* or characterisation of a candidate reference material can be done by means of an interlaboratory comparison. (See: *method performance study* and *material characterisation study*.)

Note 6: Key comparisons and supplementary comparisons are organised by the International Bureau of Weights and Measures (BIPM) in support of the International Committee for Weights and Measures (CIPM) Mutual Recognition Arrangement (MRA) in which National Metrology Institutes demonstrate the international equivalence of their *measurement standards* [VIM 5.1] and the *calibration certificates* and measurement certificates they issue [90].

Note 7: Accredited laboratories and laboratories seeking accreditation are expected to participate in interlaboratory comparisons, for example proficiency testing schemes, where available and appropriate.

Note 8: The use of terms such as “ring test”, “round robin”, “intercalibration”, “intercomparison”, “collaborative study” etc. for interlaboratory comparisons is not recommended in formal documents.

3.108 intermediate precision limit

See: *precision limit*.

3.109 internal quality control, (IQC)

Quality control within a specified laboratory.

3.110 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: [22].

3.111 laboratory information management system, (LIMS)

laboratory information system, (LIS)

Information system which can provide services to one or more *measuring systems* [VIM 3.2].

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Source: [67, 92].

Note 1: Services include the control of automated analyses, and collecting, processing, storing, and managing of data.
Note 2: LIMS functionality can include sample registration and tracking (through barcodes, chips, etc.), electronic laboratory notebooks, report generation, *quality control* and financial control.
Note 3: In laboratory medicine the term "Laboratory Information System" is common.

3.112 material characterisation study

Intralaboratory comparison or *interlaboratory comparison* with the aim of assigning a *reference quantity value* [VIM 5.18] to a *quantity* [VIM 1.1] with stated *measurement uncertainty* [VIM 2.26] or value to a reference nominal property value with stated examination uncertainty [11].

Note 1: A material characterisation study often utilizes selected (routine or reference) laboratories to measure a *candidate reference material* by *measurement procedure(s)* judged most likely to provide the smallest associated measurement uncertainty.
Note 2: Although *proficiency testing* is not primarily intended as a material characterisation study, *reference materials* are sometimes certified on the basis of results from a *proficiency testing scheme* after appropriate *quality assurance* procedures.

3.113 matrix reference material

Reference material that is characteristic of a real *sample.*

Note 1: Matrix reference materials may be obtained directly from biological, environmental, or industrial sources.
Note 2: Matrix reference materials may also be prepared by a *spike* of the *component*(s) of interest into an existing material.
Note 3: A *chemical substance* dissolved in a pure solvent is not a matrix reference material.
Note 4: Matrix reference materials are intended to be used in conjunction with the *chemical analysis* of real samples of the same or a similar *matrix*.

Source: [2].

Examples: Soil, drinking water, metal alloys, blood which fulfil the *requirements* of a reference material.

3.114 measurement capability

Ability to measure a *quantity* [VIM 1.1] in a specified interval of *quantity values* [VIM 1.19], embodied in a specified material, as demonstrated by *measurement uncertainty* [VIM 2.26].

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Note: A comparison of the measurement uncertainty in the *measurement result* [VIM 2.9] obtained by one laboratory to that of the measurement result obtained by another laboratory for the same *quantity* in the same material, compares their respective measurement capabilities.

Source: [59].

3.115 measurement precision control material

precision control material

Quality control material with or without *reference quantity value* [VIM 5.18] used in *quality control* to assess *measurement precision* [VIM 2.15].

Source: [VIM 5.13] Note 2.

3.116 measurement trueness control material

trueness control material

Quality control material with *reference quantity value* [VIM 5.18] used in *quality control* to estimate a *systematic measurement error* [VIM 2.17].

Source: [VIM 5.13] Note 2.

3.117 method performance study

Intra- or interlaboratory study of one or more *performance characteristics of a measurement method*.

Note 1: The study is normally conducted in the frame of *procedure validation* or *procedure verification*.

Note 2: Details of the *organization* and conduct of the study, for example type of *samples* and number of *measurements*, are specified in a *validation* plan or in a *protocol for interlaboratory comparison*.

Note 3: The general term "collaborative study" should not be used for an interlaboratory method performance study.

Source: [56, 93].

3.118 organization

Person or group of people that has its own functions with responsibilities, authorities and relationships to achieve its objectives.

Note 1: The concept of 'organization' includes, but is not limited to, sole-trader, company, corporation, firm, enterprise, authority, partnership, association, charity or institution, or part or combination thereof, whether incorporated or not, public or private.

Source: [61].

Note 2: In formal documents the term "body" is often used to denote an organization, for example "accreditation body", "certification body", "inspection body", "legislative body" and "regulatory body".

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3.119 out-of-control criteria

Set of decision rules for identifying the presence of special causes.

Note 1: Decision rules may include those relating to *measurement results* [VIM 2.9] inside and outside of *control limits* in a *control chart*. They cover runs, trends, cycles, periodicity, concentration of measurement results near the centre line or control limits, unusual spread of points within control limits (large or small dispersion) and relationships among values within subgroups.

Source: [4].

Note 2: Examples of decision rules and guidelines for the daily interpretation of a *control chart* are provided by Nordtest [39].

3.120 participant in an interlaboratory comparison

participant

Laboratory, *organization* or individual that receives test items and submits results for review by the *coordinator of an interlaboratory comparison*.

Source: [29].

3.121 performance characteristic of a measurement procedure

performance characteristic of a measurement method
performance characteristic

Aspect of a *measurement procedure* that may be quantitatively investigated and assessed as part of *procedure validation*.

Note 1: Performance characteristics that may be considered in procedure validation are: *analytical selectivity*, *sensitivity of a measuring system*, *working interval*, *ruggedness of a measurement procedure*, *linearity of a measuring system*, *linearity of calibration*, *critical value*, *limit of detection*, *limit of quantification*, *measurement trueness* [VIM 2.14] and *measurement precision* [VIM 2.15].

Note 2: *Measurement uncertainty* [VIM 2.26] is not a performance characteristic of a particular measurement procedure but a property of the *measurement result* [VIM 2.9] obtained using that measurement procedure.

Source: [19, 30].

3.122 performance score

performance statistic

Statistic, derived from a result reported by a *participant* in a *proficiency testing scheme*, used in interpretation of participant performance and to allow comparison with defined objectives.

Note 1: The participant result can be based on a *measurement* or an examination [11].

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Note 2: The purpose of a performance score is to express the deviation of the reported value from the *assigned value in a proficiency testing scheme* in a manner that allows comparison with performance criteria.

Note 3: Definitions and interpretations of performance scores are given in ISO/IEC 17043 [29] and ISO 13528 [27].

Table 3.122–1: Examples of performance scores used in *proficiency testing*.

Name	Symbol	Defining equation	Equation symbols
z score	z	$z_i = \frac{x_i - x_{\mathrm{PT}}}{\sigma_{\mathrm{PT}}}$	x_i: i^{th} reported value, x_{PT}: assigned value. σ_{PT}: *standard deviation for proficiency assessment.*
z' score *z prime* score	z'	$z'_i = \frac{x_i - x_{\mathrm{PT}}}{\sqrt{\sigma_{\mathrm{PT}}^2 + u^2(x_{\mathrm{PT}})}}$	$u(x_{\mathrm{PT}})$: *standard measurement uncertainty* [VIM 2.30] of the assigned value.
ζ score *zeta* score	ζ	$\zeta_i = \frac{x_i - x_{\mathrm{PT}}}{\sqrt{u^2(x_i) + u^2(x_{\mathrm{PT}})}}$	$u(x_i)$: standard measurement uncertainty of the reported value.
E_n score E_n number	E_n	$E_n(i) = \frac{x_i - x_{\mathrm{PT}}}{\sqrt{U^2(x_i) + U^2(x_{\mathrm{PT}})}}$	$U(x_{\mathrm{PT}})$: *expanded measurement uncertainty* [VIM 2.35] of the assigned value. (Usually with a *coverage probability* [VIM 2.37] of approximately 95 %). $U(x_i)$: expanded measurement uncertainty of the participant's result. (Usually with a coverage probability of approximately 95 %).

Source: [27].

3.123 precision limit

Quantity value [VIM 1.19], less than or equal to which the absolute difference between two *measured quantity values* [VIM 2.10] obtained under specified conditions of *measurement* is expected to be with a given probability.

Source: [94].

Note 1: ISO 3534-2 [4] defines three kinds of precision limit: repeatability limit (r), intermediate precision limit, and reproducibility limit (R) obtained under *repeatability conditions of measurement*, *intermediate precision conditions of measurement* [VIM 2.22], and *reproducibility conditions of measurement* [VIM 2.24], respectively. The recommended probability is 95 %.

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Note 2: Precision limit at approximately 95 % is estimated by multiplying the standard deviation obtained under the specified conditions of measurement by $2\sqrt{2}$.

3.124 procedure validation
method validation

Process of defining an analytical *requirement*, and confirming that the procedure under consideration has *capabilities* consistent with that requirement.

Note 1: Inherent in procedure validation is the need to evaluate *performance characteristics of a measurement procedure*.
Note 2: The corresponding term in ISO 15189 [54] is "validation of examination procedures".
Note 3: In ISO/IEC 17025 [22] the term "method" is used as a synonym for *measurement procedure*.
Note 4: Procedure validation is either done in a single laboratory or in the framework of an *interlaboratory comparison*.

Source: [19].

3.125 procedure verification
method verification

Confirmation, through the provision of objective evidence, that the procedure fulfils specified *requirements*.

Note 1: A laboratory that implements a procedure described in, e.g. an international standard, or in a manufacturer's documentation, needs to verify that the procedure fulfils the specified requirements.
Note 2: The corresponding term in ISO 15189 [54] is "verification of examination procedures".
Note 3: In ISO/IEC 17025 [22] the term "method" is used as a synonym for "*measurement procedure*".

Source: [19].

3.126 process in a state of statistical control
process in statistical control
stable process

Process subject only to random causes.

Note 1: The random variation is considered to follow a Gaussian distribution and is characterised by its variance (standard deviation)
Note 2: This state does not imply that the random variation is large or small, within or outside of *specification*, but rather that the variation is predictable using statistical techniques.
Note 3: A *control chart* can be used to monitor a process and to determine whether the process is, or is not, in a state of statistical control. See *out-of-control criteria* and *control limit*.

Source: [4, 21].

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3.127 proficiency test item
PT item

Sample, product, artefact, *reference material*, piece of equipment, *measurement standard* [VIM 5.1], data set or other information used for *proficiency testing*.

Source: [29].

3.128 proficiency testing, (PT)

Evaluation of the performance of a *participant in an interlaboratory comparison* against pre-established criteria.

Note 1: Proficiency testing is achieved by the distribution of representative samples for unsupervised *measurement* or examination [11] by the participants.

Note 2: Participation in *proficiency testing schemes* is not a substitute for *internal quality control* measures, or vice versa.

Note 3: The results of a participant in a proficiency testing scheme may be given as a z score, z' score, ζ score, or E_n score (see *performance score*).

Source: [29] entry 3.7.

Note 4: The term "proficiency testing" includes, but is not limited to: a) quantitative scheme — where the objective is to quantify one or more *measurands* of the *proficiency test item*; b) qualitative scheme — where the objective is to identify or describe one or more characteristics of the proficiency test item; c) sequential scheme — where one or more proficiency test items are distributed sequentially for *testing* or measurement and results returned to the *proficiency testing provider* at intervals; d) simultaneous scheme — where proficiency test items are distributed for concurrent testing or measurement within a defined time period; e) single occasion exercise — where proficiency test items are provided on a single occasion; f) continuous scheme — where proficiency test items are provided at regular intervals; g) *sampling* — where *samples* are taken for subsequent *chemical analysis*; and h) data transformation and interpretation — where sets of data or other information are furnished and the information is processed to provide an interpretation (or other outcome).

Note 5: Some proficiency testing providers in the laboratory medicine area use the term "external quality assessment (EQA)" for their proficiency testing schemes, or for their broader programmes, or both.

Source: [29].

3.129 proficiency testing provider
PT provider

Organization which takes responsibility for all tasks in the development and operation of a *proficiency testing scheme*.

Source: [29].

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3.130 proficiency testing round

PT round

Single complete sequence from distribution of *proficiency test items*, to reporting of the evaluation results to the *participants*.

Source: [29].

3.131 proficiency testing scheme

PT scheme

Proficiency testing designed and operated in one or more *proficiency testing rounds* for a specified area of testing, *measurement*, *calibration* [VIM 2.39] or *inspection*.

Note 1: A proficiency testing scheme might cover a particular type or number of tests, measurements, calibrations or inspections on *proficiency test items*.

Source: [29].

Note 2: The use of terms such as “ring test”, “round robin”, “intercalibration”, “intercomparison”, “collaborative study” etc. for proficiency testing schemes is not recommended in formal documents.

3.132 protocol for interlaboratory comparison

Detailed set of instructions describing the objectives, design, conduct, and reporting of an *interlaboratory comparison*.

3.133 quality

Degree to which a set of inherent characteristics of an object fulfils *requirements*.

Note 1: The term “quality” can be used with adjectives such as poor, good or excellent.

Note 2: “Inherent”, as opposed to “assigned”, means existing in the object.

Source: [61].

Note 3: *Measurement uncertainty* [VIM 2.26] provides a quantitative measure of the quality of a *measurement result* [VIM 2.9].

3.134 quality assurance, (QA)

Part of *quality management* focused on providing confidence that specified *requirements* for *quality* will be fulfilled.

Source: [61]. Entry replaces recommendation in [20] p 2208.

3.135 quality control, (QC)

Part of *quality management* focused on fulfilling specified *requirements* for *quality*.

Source: [61]. Entry replaces recommendation in [95] p 1535, [20] p 2208.

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3.136 quality control material
control material

Material used for the purposes of *quality control* and subjected to the same or part of the same *measurement procedure* as that used for *analytical samples*.

Note 1: *Blank materials, analytical samples*, *reference materials* and *certified reference materials* [VIM 5.14] can be used as quality control materials.
Note 2: Nordtest [80] p 13, advises that for *Shewhart range charts* the best samples to be used are test samples selected from among the samples to be analysed in that analytical run.

Source: [80, 96].

3.137 quality improvement

Part of *quality management* focused on increasing the ability to fulfil *requirements* for *quality*.

Note: The requirements can be related to any aspect such as effectiveness, efficiency or *object traceability*.

Source: [61].

3.138 quality management

Coordinated activities to direct and control an *organization* with regard to *quality*.

Note: Quality management can include establishing *quality policies* and *quality objectives*.

Source: [61].

3.139 quality management system

Part of a set of interrelated or interacting elements of an *organization* to establish *quality policies* and *quality objectives*, and processes to achieve those objectives.

Source: [61].

Note 1: A laboratory's structure, roles and responsibilities, planning, operation, practices, rules, and beliefs are also established within the quality management system.
Note 2: Other common parts of a laboratory's management system are financial management and environmental management.

3.140 quality manual

Specification for the *quality management system* of an *organization*.

Note: Quality manuals can vary in detail and format to suit the size and complexity of an individual *organization*.

Source: [61].

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3.141 quality objective

Result to be achieved related to *quality*.

Note 1: Quality objectives are generally based on the *quality policy* of the *organization*.

Note 2: Quality objectives are generally specified for relevant functions, levels and processes in the organization.

Source: [61].

Note 3: In the context of *quality management systems* quality objectives are set by the laboratory, consistent with the quality policy, to achieve specific results.

3.142 quality plan

Specification of the procedures and associated resources to be applied when and by whom to a specific object.

Note 1: These procedures generally include those referring to *quality management* processes and to product and service realization processes.

Note 2: A quality plan often makes reference to parts of the *quality manual* or to procedure documents.

Note 3: A quality plan is generally one of the results of *quality planning*.

Source: [61].

3.143 quality planning

Part of *quality management* focused on setting *quality objectives* and specifying necessary operational processes, and related resources to achieve the *quality objectives*.

Note: Establishing *quality plans* can be part of quality planning.

Source: [61].

3.144 quality policy

Intentions and direction of a laboratory as formally expressed by its top management related to *quality*.

Note: Generally, the quality policy is consistent with the overall policy of the laboratory, can be aligned with the laboratory's vision and mission and provides a framework for the setting of *quality objectives*.

Source: [61].

3.145 reference laboratory

Laboratory that applies a *reference measurement procedure* [VIM 2.7], a reference examination procedure [11] or performs a *calibration* [VIM 2.39].

Note 1: The term "reference laboratory" may have other connotations in a national context.

Note 2: In laboratory medicine a reference measurement laboratory is defined in ISO 15195:2003 [70].

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3.146 reference material, (RM)

Material, sufficiently homogeneous and stable with reference to specified properties, which has been established to be fit for its intended use in *measurement* or in examination of *nominal properties* [VIM 1.30].

Note 1: Examination of a nominal property provides a nominal property value and associated examination uncertainty.

Note 2: Reference materials with or without assigned *quantity values* [VIM 1.19] can be used for *measurement precision* [VIM 2.15] control whereas only reference materials with assigned quantity values can be used for *calibration* [VIM 2.39] or *measurement trueness* [VIM 2.14] control.

Note 3: 'Reference material' comprises materials embodying *quantities* [VIM 1.1] as well as nominal properties.

Example 1: Examples of reference materials embodying quantities:
a) water of stated purity, the dynamic viscosity of which is used to calibrate viscometers;
b) human serum without an assigned quantity value for the amount-of-substance concentration of the inherent cholesterol, used only as a *measurement precision control material*;
c) fish tissue containing a stated mass fraction of a dioxin, used as a *calibrator* [VIM 5.12].

Example 2: Examples of reference materials embodying nominal properties:
a) colour chart indicating one or more specified colours;
b) DNA compound containing a specified nucleotide sequence;
c) urine containing 19-androstenedione.

Note 5: Some reference materials have assigned quantity values that are metrologically traceable to a *measurement unit* [VIM 1.9] outside a *system of units* [VIM 1.13]. Such materials include vaccines to which International Units (IU) have been assigned by the World Health Organization.

Note 6: In a given measurement, a given reference material can only be used for either *calibration* [VIM 2.39] or *quality assurance*.

Note 7: The specifications of a reference material should include its material traceability, indicating its origin and processing [97].

Source: [VIM 5.13] with Notes 4 and 8 omitted. See also: *material stability*, *material homogeneity*, *fitness for purpose*. For Note 1 see [11] entry 3.9. For Note 2 see also: *property value assignment*, *conventional quantity value*, *measurement trueness control material*. For Note 3 Example 1a see *chemical purity*. For Note 7 see also *object traceability*.

Note 9: The "product information sheet" is a document containing all the information that is essential for using a reference material [2].

Note 10: Good practice in using reference materials and *certified reference materials* [VIM 5.14], in particular in measurement processes, is described in ISO Guide 33 [96].

Entry replaces recommendation in [20] p 2210.

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3.147 reference material certificate

Document, issued by a *reference material producer*, containing the essential information for the use of a *certified reference material* [VIM 5.14] and confirming that the necessary procedures have been carried out to ensure the validity and traceability of the stated property values.

Note 1: A reference material certificate is usually valid for a stated period of time ("period of validity" or as described by its "expiry date") which defines the *shelf life* of the certified reference material.

Note 2: Documents containing the information described above, may for legal or other (non-technical) reasons not be termed "certificate" (compare Note 1 to certified reference material).

Note 3: ISO Guide 31 [60] is the guidance document to the required and recommended content of a reference material certificate.

Source: [2, 47, 60].

Note 4: In this definition, "traceability" covers both '*metrological traceability*' [VIM 2.41] of a *measurement result* [VIM 2.9] and examination traceability [11] but not *object traceability*.

3.148 reference material certification

certification of a reference material

Process that formally establishes the *certified property value*(*s*) of a *candidate certified reference material*.

Note 1: The process is the responsibility of the *reference material producer*.

Note 2: Properties of a material include qualitative properties such as identities of *chemical substances*, and quantitative properties such as mass concentration.

Note 3: The outcome of the process is *a reference material certificate*.

Note 4: Reference material certification is a "first-party attestation" in accordance with the definition of the term "declaration" (See [64] section 5.4).

Source: [2].

3.149 reference material certification report

certification report

Document giving detailed information, in addition to that contained in a *reference material certificate*.

Note: The information may refer to, e.g. the preparation of the *reference material*, *measurement procedures*, factors affecting *measurement accuracy* [VIM 2.13], statistical treatment of *measurement results* [VIM 2.9], and the way in which *metrological traceability* [VIM 2.41] was established.

Source: [2, 47, 60].

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3.150 reference material producer
RM producer

Technically competent body, that produces a *reference material* compliant with the appropriate guidance documents and issues the reference material documentation.

Note 1: The reference material producer may be an *organization* or company, public or private.
Note 2: The relevant guidance documents are the ISO Guides 31 [60] and 35 [47]..
Note 3: ISO 17034 [50] provides the general *requirements* for the *competence* of reference material producers.

Source: [2].

3.151 rejection interval
rejection zone

Interval of non-permissible *measured quantity values* [VIM 2.10].

Note: Non-permissible measured quantity values are associated with items that do not conform to a *specification* and lie outside the *acceptance interval*.

Source: [68, 69]. See also *conformity assessment*.

3.152 repeatability limit, *r*
See: *precision limit*.

3.153 reproducibility limit, *R*
See: *precision limit*.

3.154 requirement

Need or expectation that is stated, generally implied or obligatory.

Note 1: "Generally implied" means that it is custom or common practice for the *organization* and interested parties that the need or expectation under consideration is implied.
Note 2: A specified requirement is one that is stated, for example in documented information.

Source: [61].

3.155 ruggedness of a measurement procedure
robustness of a measurement procedure

Ability of a *measurement procedure* to maintain acceptable performance under minor changes in operating conditions.

Note 1: Ruggedness is normally investigated as part of procedure development and may be part of *procedure validation*.
Note 2: The outcome of a ruggedness *test* provides objective evidence of the applicability of the measurement procedure during normal usage.

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Note 3: A measurement procedure, the performance of which remains unaffected by minor changes in operating conditions, is usually said to be "rugged" or "robust".

Source: [19].

3.156 sensitivity of a measuring system

analytical sensitivity
sensitivity

Quotient of the change in an *indication* [VIM 4.1] of a *measuring system* [VIM 3.2] and the corresponding change in a *quantity* [VIM 1.1] being measured.

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

Note 2: The change considered in a value of a quantity being measured must be large compared with the *resolution* [VIM 4.14].

Source: [VIM 4.12].

Note 3: Sensitivity of a measuring system can be obtained from the slope of the *calibration curve*.

Note 4: Sensitivity of a measuring system should not be confused with diagnostic sensitivity in laboratory medicine.

Note 5: Sensitivity of a measuring system should not be confused with *limit of detection* or *limit of quantification*.

See [19]. Entry replaces recommendation in [20] p 2167. See also: *analytical sensitivity*, *selectivity of a measuring system* [VIM 4.13].

3.157 Shewhart control chart

Control chart 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.

Source: [4]. See also [81].

3.158 Shewhart control limit

Control limit determined statistically from the variation of the process due to random causes alone.

Source: [79]. See also [81].

3.159 Shewhart means chart

Shewhart control chart in which the means of *measured quantity values* [VIM 2.10] are plotted against time.

Example: A Shewhart means chart with mean values from a *process in a state of statistical control* with a simulated change in the process mean after 10 days is shown in Figure 3.159-1.

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Note 1: Nordtest [80] terms a control chart with *measured quantity values* [VIM 2.10] scaled by the mean or target value an "X-chart". ISO uses the term "*X*-control chart" for a control chart which plots single values [79] entry 3.17.

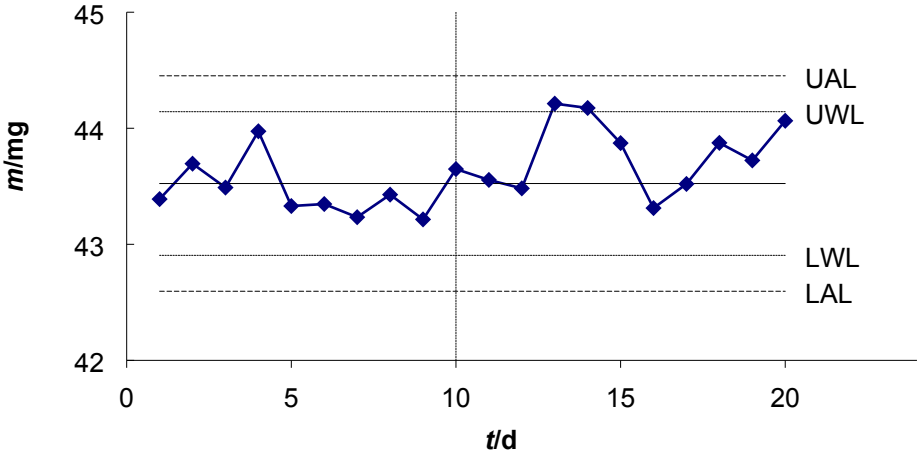

Figure 3.159-1. Shewhart means chart of the means of duplicate analyses of a *quality control material*, twice per day (d) over 20 days. Each point is the mean of the day's four results ($n = 4$). Upper and lower warning limits (UWL, LWL) are at $\bar{x} \pm 2s/\sqrt{n}$ where $\bar{x}$ is the process mean, s is the standard deviation under *repeatability conditions of measurement*, and upper and lower action limits (UAL, LAL) are at $\bar{x} \pm 3s/\sqrt{n}$. A simulated *measurement bias* [VIM 2.18] of one standard deviation is applied after day 10.
Source: [81].

3.160 Shewhart range chart

Shewhart control chart in which the ranges of *measured quantity values* [VIM 2.10] are plotted against time.

Note 1: The range is the greatest measured quantity value minus the least measured quantity value.

Note 2: Warning and action limits are given in tables (e.g. [81] 6.1) as a function of the number of measured quantity values (n) taken to obtain the range and of the expected average range.

Source: [81].

3.161 specification

Expression of permissible limits on a characteristic.

Source: [98].

3.162 standard deviation for proficiency assessment, σ_{PT}

Measure of dispersion used in the evaluation of results of *proficiency testing*.

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Note: Not all *proficiency testing schemes* evaluate proficiency based on the dispersion of results.

Source: [27].

3.163 standard operating procedure, (SOP)
recommended operating procedure, (ROP)
standard method

Authorized, documented procedure or set of procedures with detailed instructions for specified activities.

Note: Laboratory activities for which standard operating procedures are issued include *sampling*, *measurement*, *testing* and examination [11].

Source: [99].

3.164 statistical process control, (SPC)

Activities focused on the use of statistical techniques to reduce variation, increase knowledge about the process and steer the process in the desired way.

Note: Although statistical process control originally was concerned primarily with manufactured goods, it is also equally applicable to processes producing services, for example a *measurement procedure*.

Source: [4].

3.165 target measurement uncertainty
target uncertainty

measurement uncertainty [VIM 2.26] specified as an upper limit and decided on the basis of the intended use of *measurement results* [VIM 2.9].

Source: [VIM 2.34].

Note: Setting and using target uncertainty is described in [100].

3.166 tolerance
specified tolerance

Difference between upper and lower *tolerance limits*.

Source: [69]. See also *conformity assessment*.

Note: Tolerance should not be confused with *measurement uncertainty* [VIM 2.26].

3.167 tolerance interval
specification zone

Interval of permissible *quantity values* [VIM 1.19].

Note 1: Unless otherwise stated in a *specification*, the *tolerance limits* belong to the tolerance interval.

Note 2: The term “tolerance interval” as used in *conformity assessment* has a different meaning from the same term as it is used in statistics.

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Source: [68, 69]. See also *conformity assessment*.

3.168 tolerance limit

specification limit

Specified upper or lower bound of permissible *quantity values* [VIM 1.19].

Source: [69] 3.3.4. See also *conformity assessment*.

3.169 total quality management, (TQM)

Organization-wide efforts to install a permanent climate in which an organization continuously improves its ability to deliver high-*quality* products and services to customers.

Source: [83].

3.170 validation

Confirmation, through the provision of objective evidence, that the *requirements* for a specific intended use or application have been fulfilled.

Note 1: The objective evidence needed for a validation is the result of a *test* or other form of *determination* such as performing alternative calculations or reviewing documents.

Note 2: The term "validated" is used to designate the corresponding status.

Note 3: The use conditions for validation can be real or simulated.

Source: [61].

Note 4: In the VIM [1] 'validation' as "verification, where the specified requirements are adequate for an intended use".

3.171 verification

Confirmation, through the provision of objective evidence, that specified *requirements* have been fulfilled.

Note 1: The objective evidence needed for a verification can be the result of an *inspection* or of other forms of *determination* such as performing alternative calculations or reviewing documents.

Note 2: The activities carried out for verification are sometimes termed "qualification process".

Note 3: The word "verified" is used to designate the corresponding status.

Source: [61].

Note 4: In the VIM [1] 'verification' is defined as "provision of objective evidence that a given item fulfils specified requirements".

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3.172 Youden plot

Graphical technique for evaluating an *interlaboratory comparison* when each *participant* has made two *measurements* on the same *sample* or one measurement on each of two different samples.

Note 1: The coordinates of each point may be the *measured quantity values* [VIM 2.10] themselves or any transformation thereof such as a *performance score*, for example a *z* score. (See Figure 3.172-1).

Note 2: The Youden plot is a simple but effective method for comparing both within-laboratory variability and between-laboratory variability.

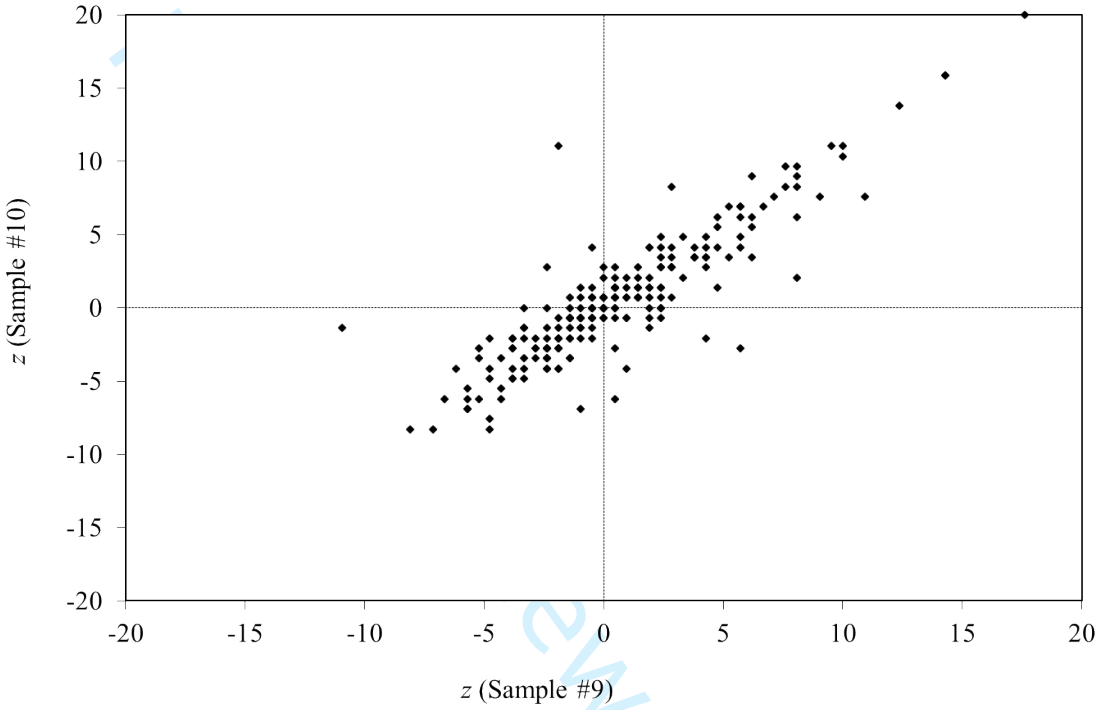

Figure 3.172-1. Youden plot of the *z* scores of samples #9 and #10 of Round 5 of U39 of the *proficiency testing* program held by the RCPA Australia for the analysis of creatinine in urine by 218 laboratories. (Reproduced from [101] with permission).

4 INDEX OF SYMBOLS AND ABBREVIATIONS

σ_{PT}	standard deviation for proficiency assessment
ζ	*zeta* score
E_n	E_n score
H	Horwitz ratio
L_c	critical value
r	repeatability limit. See: *precision limit*.

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R	reproducibility limit. See: *precision limit*.
$s_{R,H}$	reproducibility standard deviation estimated by the *Horwitz equation*
z	z score
z', z-prime	z' score
CUSUM	cumulative sum
DL	detection limit. See: *limit of detection*.
GLP	good laboratory practice
GMP	good manufacturing practice
Horrat (HorRat, HORRAT)	Horwitz ratio
ILC	interlaboratory comparison
IQC	internal quality control
LCL	lower action limit. See: *control limit*.
LIMS	laboratory information management system
LIS	laboratory information system
LLOQ	lower limit of quantification. See: *limit of quantification*.
LOD	limit of detection
LOQ	limit of quantification
LWL	lower warning limit. See: *control limit*.
PT	proficiency testing
QA	quality assurance
QC	quality control
RM	reference material
ROP	recommended operating procedure. See: *standard operating procedure*.
SOP	standard operating procedure
SPC	statistical process control
TQM	total quality management
UCL	upper action limit. See: *control limit*.
ULOQ	upper limit of quantification. See: *limit of quantification*.
UWL	upper warning limit. See: *control limit*.
VIM	International vocabulary of metrology, 3rd edition.[1]

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