

Fundamental and Metrological Concepts in Analytical Chemistry^{†,‡}

1.1 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, in *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, this chapter aims at providing such concepts and terms to complement VIM in the field of analytical chemistry. Hopefully, this will contribute to focusing their current usage and stabilizing their consistent application.

The majority of terms in this chapter have been published as an IUPAC Recommendation “Metrological and Quality Concepts in Analytical Chemistry”² and where no change is indicated, this is the source of an entry without further reference. Entries based on VIM are referenced as “Source: [VIM n.m]” where n.m is the VIM concept number. The VIM definition, where given, is not changed (other than to satisfy the formatting of this chapter) although not all notes and examples are reproduced. These are denoted as “with Note xx omitted”. Further notes to clarify chemical usage may be given after the VIM text. In the text of an entry VIM references are given in the usual format.¹ For non-VIM sources the respective reference number (*e.g.*, “See also: ref. 3” for ISO Guide 30) is used in the sense that information is taken from there. Where an entry from ref. 2 replaces that in a previous Recommendation, or the previous edition of the Orange Book,⁴ the earlier version is not referenced here, but can be found in the respective previous issue.

Compliance with the norms issued by the 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”, and “mass concentration” are used to identify both specific concepts

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[‡]IUPAC contact for this chapter: Dr Ernst-Heiner Korte, ISAS, Bunsen-Kirchhoff-Str. 11, 44139 Dortmund, Germany. h.korte@acqual.de.

under ‘quantity’ [VIM 1.1] (Note 1) and ‘kinds-of-quantity’ [VIM 1.2] (Note 3). While in laboratory medicine⁵ these concepts are termed ‘kinds of quantity’ throughout, we will follow the usage of the Green Book,⁶ the *International System of Quantities (ISQ)* [VIM 1.6] *etc.* to refer to them as ‘quantities’. Following the VIM convention double quotation marks are used around terms and direct quotes, and single quotation marks are used around concepts.

1.2 Definitions of Analytical Chemistry

The discipline of analytical chemistry aims at obtaining knowledge about matter by examining its properties. This Chapter 1 strives to cover all types of properties whether unitary, ordinal, or nominal (see Section 1.3): as defined below quantitative analysis results in measured quantity values, while qualitative analysis is the *examination* of a material.

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”.⁷

Note 2: The term “analytical science” was coined in 1998 to emphasise the impact of informatics on analytical chemistry.⁸

See also: ref. 7, *chemical analysis*.

1.2 chemical analysis

Application of *analytical chemistry*.

See also: ref. 7.

1.3 qualitative analysis

qualitative examination

Examination of nominal properties in analytical chemistry.

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

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

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

1.4 quantitative analysis

Measurement in analytical chemistry.

Note: Quantitative analysis is used to obtain *quantity values* for *ordinal quantities* and *unitary quantities*.

1.3 Concepts used in Laboratory Practice

1.5 additive matrix effect

Matrix effect that is independent of the *quantity value* of the *measurand*.

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”.⁹

Example 1: An additive matrix effect that originates from a missing or flawed *blank correction*.¹⁰

Example 2: The measurement of plutonium mass concentration using a K-edge densitometer in the presence of a uranium admixture. The presence of uranium causes a large additive matrix effect.¹¹

1.6 aliquot

specimen

Portion of a material assumed to be taken with negligible sampling error.¹²

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

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

1.7 analyte*Component* specified in a *measurand*.

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

Note 2: A component to be identified by *examination* should not be termed analyte but ‘examinand’.¹³

1.8 analytical run

run

Set of *measurements* of the same *quantity* 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*.

See also: ref. 14.

1.9 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 can be considered to be the combination of an *analyte* and a *matrix*.

Note 2: A portion of the analytical sample may be termed an *aliquot* if it is taken with negligible sampling error.¹²

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

Note: In VIM 4.2, this concept is termed “blank indication” with “background indication” as an 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: definition from [VIM 4.2], with added Note.

1.11 batch

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

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

1.12 blank correctionStep in a *measurement procedure* in which the effect of a *blank indication* is removed from an *indication*.

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

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.

1.13 blank indication

Indication obtained from a sample of *blank material* under the same 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. See ref. 4 p. 44 of Section 18.

See: *background indication*.

1.14 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 blanks are nearly always an essential part of *chemical analysis* and may be part of *quality assurance* and *quality control*. See ref. 15 p. 130.

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 material type of blank.

Note 4: The term “procedure (or procedural) 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 procedure.

Note 5: A blank 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 the blank indication or the related *blank value* or *blank correction*, this must be clarified by the context.

See also: ref. 14 and 15. Source: ref. 2 entry 3.15 with amended Note 4.

1.15 blank value

Measured quantity value obtained by application of the *calibration function* to the *blank indication*.

Note: The concepts ‘blank value’ and ‘blank indication’ should not be confused.

1.16 chemical purity

purity

Mass (amount of substance or number of entities) of a specified *component* divided by the mass (amount of substance or 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*, component and system must be specified.

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

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

1.17 chemical substance

substance

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

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

1.18 component

Part of a *system*.

Note 1: A component can consist of different chemical species.

Note 2: “Part” is not to be taken for an *aliquot* or a portion or a *sample* of a system.

Note 3: The concept ‘component’ is likewise used with “material”, “matter” and “substance”.

Source: ref. 2 entry 3.24 with added Note 3. See also: ref. 16.

1.19 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*, and so, the term “determination” should not be used when “measurement” or “examination” applies.

Note 3: ISO 9000 defines “determination” as “activity to find out one or more characteristics and their characteristic values”.¹⁷

See also: ref. 18 section 3.11.1, *testing*.

1.20 interference

Process whereby a *measured quantity value* is changed by an *influence quantity*.

1.21 interferent

Component of the *matrix* that embodies an *influence quantity*.

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 $^{40}\text{Ar}^{35}\text{Cl}^+$ which has the same *m/z* value as As^+ (*m/z* 75).

1.22 internal standard

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

Note 1: An internal standard provides an *indication* 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* 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*.

1.23 isotopic purity

Amount-of-substance fraction of a specified *nuclide* among all nuclides of the same element.

Source: ref. 19.

1.24 laboratory sample

Sample or a subsample sent to or received by a laboratory.

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

See also: ref. 12. See also: *primary sample*, *aliquot*, *sampling plan*, and *sample pre-treatment*.

1.25 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 the 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 11961,²⁰ ISO 472,²¹ ISO 15736,²² and ISO 18113-1.²³

1.26 mass balance

See: *chemical purity*.

1.27 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* if the *quantity values* measured using specified *aliquots* of the material aliquots of a 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 (termed “between-bottles homogeneity” or “within-bottle homogeneity”, respectively).

Note 3: Inhomogeneity is a source of *measurement uncertainty*.

Note 4: Detailed guidance for the assessment of homogeneity of *reference materials*, is given in ISO Guide 35.²⁴

1.28 material measure

Measuring instrument reproducing or supplying, in a permanent manner during its use, *quantities* of one or more given *kinds*, each with an assigned quantity value.

Example: Standard weight, volume measure (supplying one or several quantity values, with or without a quantity-value scale), standard electric resistor, line scale (ruler), gauge block, standard signal generator, *certified reference material*.

Note 1: The *indication* of a material measure is its assigned quantity value.

Note 2: A material measure can be a *measurement standard*.

Source: [VIM 3.6]. See also: *property value assignment*, *conventional quantity value*.

1.29 material recovery

recovery

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

Note 1: The *measurement unit* of material recovery is the measurement unit of the *quantity* 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.

1.30 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 or examined 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”).

See: ref. 3 Section 2.1.

Note 3: The variation of the property value over time adds a contribution to the *uncertainty budget* or the *examination uncertainty*, as applicable. Regarding the assessment of stability of *reference material*, detailed guidance is given in ISO Guide 35.²⁴

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

1.31 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.

1.32 matrix effect

Systematic measurement error caused by the *matrix*.

See also: *multiplicative matrix effect*, *additive matrix effect*

1.33 multiplicative matrix effect

Matrix effect that is proportional to the *measured quantity value* 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”.⁹

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

1.34 primary sample

Collection of one or more sampling increments² initially taken from material intended to be analysed.

Note: 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: ref. 12 Appendix B.

1.35 recovered quantity value ratio, *R*

analytical recovery

recovery

Measured quantity value relating a *component* to a *system* divided by a *reference value*.

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

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

Note 3: The definition can be symbolized by $R_B = Q_{B,\text{measured}}/Q_{B,\text{reference}}$, where *R* denotes the recovered ratio of the *quantity values* *Q*, and B indicates 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: Recovered quantity value ratio is used in *procedure validation*¹⁴ to evaluate and correct for the *measurement procedure bias*.

Note 6: Recovered quantity value ratio may be estimated from the measured change of the quantity value of the component of interest upon the 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*, and *spike*.

See also: ref. 14 and 25.

1.36 replicate (duplicate) sample

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

Note 1: This selection may be accomplished by taking sampling increments² 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.

Note 2: In ISO 3534-2, ‘replicate sampling’ is defined (see ref. 26 entry 5.2.5).

1.37 sample

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

Note 1: Taking a sample from a larger amount of material implies the existence of a sampling error,¹² *i.e.*, the *measured quantity values* 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 preparation in *analytical chemistry* are detailed in ref. 27 and 28.

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.

See also: *analytical sample*, *laboratory sample*, *primary sample*, *replicate sample*, and *spike*.

1.38 sample pre-treatment

sample preparation

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

Note: Sample pre-treatment includes, *e.g.*, mixing, splitting, drying, crushing, stabilization, dissolving, *extraction*, diluting, precipitating, and derivatizing.

See also: ref. 29 Appendix B, Chapter 3.

1.39 sampling

Act of taking or constituting a *sample*.

Note: Sampling often provides a contribution to the *measurement uncertainty budget* or the *examination uncertainty*, as applicable. See: ref. 12.

See also: ref. 26.

1.40 sampling plan

Predetermined procedure for the selection, withdrawal, preservation, transportation and preparation (see *sample pre-treatment*) of the portions to be removed from a material as a *sample*.

See also: ref. 12 Appendix B.

1.41 sampling target

Portion of the 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).

See also: ref. 12 Appendix B. Source: ref. 2 entry 3.70 with minor amendment.

1.42 spike

Material with known *quantity values* added to an *analytical sample*.

Note 1: The material can be a *reference material* or a *certified reference material*.

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*.

Note 4: “Spike” used as a verb is the addition of a spike to a *sample*.

1.43 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.

Note: The concept covers both immaterial systems such as the *International System of Units* and material systems such as a *measuring system*. In laboratory medicine, the term “system” usually denotes a composite object such as a living organism or tissue;⁵ in *analytical chemistry*, the term is used to emphasize complex interaction of components.

Example 1: The tailings dam of a mine containing water and unknown amounts of 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*.

See also: ref. 16. Source: ref. 2 entry 3.73 with minor amendment.

1.4 Concepts Related to Properties, Quantities And Units

The concepts defined in *analytical chemistry*, as well as in many other disciplines, are related to the properties used for description of objects and *examinations* and *measurements* applied to obtain their nominal property values and *measured quantity values* respectively. The superordinate concept ‘property’ can be divided into subordinate specific concepts by applying the division criterion ‘allowable algebraic comparisons between individual properties having the same kind of property’. See Table 1.1.

The ensuing specific concepts can be arranged into a generic concept system, here as an indented list in the left column of Table 1.1. Allowable comparisons for four salient types of property are given in the second column.

The term “qualitative property” is often seen, but unfortunately with two meanings: either ‘*nominal property*’ or both ‘*nominal property*’ and ‘*ordinal quantity*’. The term “quantitative property” sometimes includes ‘*ordinal quantities*’, sometimes not. Such problems are avoided by using the systematic terms given in Table 1.1.

Table 1.1 Generic concept system on ‘property’. The letters a , b , c , and d signify individual properties in comparisons; n is a numerical factor.

Type of property	Allowable comparison	Example
nominal property	$a = b$ $a \neq b$	colour
quantity ordinal quantity	$a < b$ $a = b$ $a > b$ $a \neq b$	octane number
unitary quantity differential (unitary) quantity	$ a - b = c - d $ $ a - b \neq c - d $	Celsius temperature, pH
rational (unitary) quantity	$a = n \times b$ $a \neq n \times b$	mass, thermodynamic temperature

1.44 base quantity

Quantity in a conventionally chosen subset of a given *system of quantities*, where no subset quantity can be expressed in terms of the others.

Note 1: The subset mentioned in the definition is termed the “set of base quantities”.

Example: The set of base quantities in the *International System of Quantities* (ISQ).

Note 2: Base quantities are referred to as being mutually independent since a base quantity cannot be expressed as a product of powers of the other base quantities.

Note 3: ‘Number of entities’ can be regarded as a base quantity in any system of quantities.

Source: [VIM 1.4].

1.45 base unit

Measurement unit that is adopted by convention for a *base quantity*.

Note 1: In each *coherent system of units*, there is only one base unit for each base quantity.

Example: In the *SI*, the metre is the base unit of length. In the CGS systems, the centimetre is the base unit of length.

Note 2: A base unit may also serve for a *derived quantity* of the same *quantity dimension*.

Example: Rainfall, when defined as areic volume (volume per area), has the metre as a *coherent derived unit* in the *SI*.

Note 3: For number of entities, the number one, symbol 1, can be regarded as a base unit in any *system of units*.

Source: [VIM 1.10].

1.46 coherent derived unit

Derived unit that, for a given *system of quantities* and for a chosen set of *base units*, is a product of powers of base units with no other proportionality factor than one.

Note 1: A power of a base unit is the base unit raised to an exponent.

Note 2: Coherence can be determined only with respect to a particular system of quantities and a given set of base units.

Examples: If the metre, the second, and the mole are base units, the metre per second is the coherent derived unit of velocity when velocity, v , is defined by the quantity equation $v = dr/dt$ where r denotes distance and t time, and the mole per cubic metre is the coherent derived unit of amount-of-substance concentration when amount-of-substance concentration, c , is defined by the quantity equation $c = n/V$ where n

denotes amount of substance and V volume. The kilometre per hour and the knot are examples of derived units which are not coherent derived units in the *International System of Quantities*.

Note 3: A derived unit can be coherent with respect to one system of quantities, but not to another.

Example: The centimetre per second is the coherent derived unit of speed in the CGS *system of units* but is not a coherent derived unit in the *SI*.

Note 4: The coherent derived unit for every derived *quantity of dimension one* in a given system of units is the number one, symbol 1. The name and symbol of the *measurement unit one* are generally not indicated.

Source: [VIM 1.12].

1.47 coherent system of units

System of units, based on a given *system of quantities*, in which the *measurement unit* for each *derived quantity* is a *coherent derived unit*.

Example: Set of coherent *SI* units and relations between them.

Note 1: A system of units can be coherent only with respect to a system of quantities and the adopted *base units*.

Source: [VIM 1.14] with Note 2 omitted.

1.48 conventional quantity value

conventional value of a quantity

conventional value

Quantity value attributed by agreement to a *quantity* for a given purpose.

Example 3: Conventional quantity value of a given mass standard, $m = 100.00347$ g.

Note 2: Sometimes a conventional quantity value is an estimate of a *true quantity value*.

Note 3: A conventional quantity value is generally accepted as being associated with a suitably small *measurement uncertainty*, which might be zero.

Example 4: Relative atomic mass for carbon as listed in the IUPAC Green Book.⁶

Example 5: *Consensus property value* of the *measured values* of an *interlaboratory comparison*³⁰ entry 3.11.

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*”.

Source: [VIM 2.12] with Note 1 and Examples 1 and 2 omitted, and Examples 4 and 5 and Note 4 added.

1.49 derived quantity

Quantity, in a *system of quantities*, defined in terms of the *base quantities* of that system.

Example: In a system of quantities having the base quantities length and mass, mass density is a derived quantity defined as the quotient of mass and volume (length to the third power).

Source: [VIM 1.5].

1.50 derived unit

Measurement unit for a *derived quantity*.

Example: The metre per second, symbol m/s, and the centimetre per second, symbol cm/s, are derived units for speed in the *SI*. The kilometre per hour, symbol km/h, is a measurement unit for speed outside the *SI* but accepted for use with the *SI*. The knot, equal to one nautical mile per hour, is a measurement unit of speed outside the *SI*.

Source: [VIM 1.11].

1.51 International System of Quantities, (ISQ)

System of quantities based on the seven *base quantities*: length, mass, time, *electric current*, thermodynamic temperature, amount of substance, and luminous intensity.

Note 1: This system of quantities is published in the ISO 80000 series Quantities and units.³¹

Note 2: The *International System of Units* is based on the ISQ.

Source: [VIM 1.6].

1.52 International System of Units, (SI)

System of units, based on the *International System of Quantities*, their names and symbols, including a series of prefixes and their names and symbols, together with rules for their use, adopted by the General Conference on Weights and Measures (CGPM).

Note 1: The SI is founded on the seven *base quantities* of the ISQ and the terms and symbols of the corresponding *base units* that are contained in Table 1.2.

Note 2: The base units and the *coherent derived units* of the SI form a coherent set, designated the “set of coherent SI units”.

Note 3: For a full description and explanation of the International System of Units, see the current edition of the SI brochure published by the Bureau International des Poids et Mesures (BIPM)³² and available on the BIPM website.³³

Note 4: In *quantity calculus*, the quantity ‘number of entities’ is often considered to be a base quantity, with the base unit ‘one’, symbol ‘1’.

Note 5: SI prefixes for multiples of units and submultiples of units are given in Table 1.3.

Note 6: The SI prefixes given in Table 1.3 may be used for decimal multiples and decimal submultiples of SI base units and SI derived units only. The prefixes refer strictly to powers of 10 and should not be used for powers of 2 for which other prefixes apply. A non-decimal multiple of the SI base unit second is the hour. See: ref. 1 entry 1.17.

Note 7: From 20 May 2019, SI units are based on seven “defining constants” the numerical values of which are fixed.³² The constants are: the hyperfine transition *frequency* of the caesium 133 atom, the speed of light in vacuum, the Planck constant, the elementary charge, the Boltzmann constant, the Avogadro constant, and the luminous efficacy of monochromatic radiation of frequency 540×10^{12} Hz. These constants are defined and so have no uncertainty. See Table 1.9.

Source: [VIM 1.16] with added Notes 6 and 7.

Table 1.2 Base quantities of the International System of Quantities and their corresponding SI base units.

Base quantity	Base unit	
Term	Term	Symbol
length	metre	m
mass	kilogram	kg
time	second	s
<i>electric current</i>	ampere	A
thermodynamic temperature	kelvin	K
amount of substance	mole	mol
luminous intensity	candela	cd

Table 1.3 SI prefixes of units.

Factor	Name	Symbol
10^{24}	yotta	Y
10^{21}	zetta	Z
10^{18}	exa	E
10^{15}	peta	P
10^{12}	tera	T
10^9	giga	G
10^6	mega	M
10^3	kilo	k
10^2	hecto	h
10^1	deka	da
10^{-1}	deci	d
10^{-2}	centi	c
10^{-3}	milli	m
10^{-6}	micro	μ
10^{-9}	nano	n
10^{-12}	pico	p
10^{-15}	femto	f
10^{-18}	atto	a
10^{-21}	zepto	z
10^{-24}	yocto	y

1.53 kind of quantity

kind

Aspect common to mutually comparable *quantities*.

Note 1: The division of 'quantity' according to 'kind of quantity' is to some extent arbitrary.

Example 1: The quantities diameter, circumference, and *wavelength* are generally considered to be quantities of the same kind, namely of the kind of quantity termed length.

Example 2: The quantities heat, kinetic energy, and potential energy are generally considered to be quantities of the same kind, namely of the kind of quantity termed energy.

Note 2: Quantities of the same kind within a given *system of quantities* have the same *quantity dimension*. However, quantities of the same dimension are not necessarily of the same kind.

Example: The quantities moment of force and energy are, by convention, not regarded as being of the same kind, although they have the same dimension. Similarly for heat capacity and entropy, as well as for number of entities, relative permeability, and mass fraction.

Note 3: In English, the terms for quantities in the left half of Table 1.4, are often used for the corresponding 'kinds of quantity'.

Source: [VIM 1.2].

1.54 measurement unit

unit of measurement

unit

Real scalar *quantity*, defined and adopted by convention, with which any other quantity of the same *kind* can be compared to express the ratio of the two quantities as a number.

Note 1: Measurement units are designated by conventionally assigned names and symbols.

Note 2: Measurement units of quantities of the same *quantity dimension* may be designated by the same term and symbol even when the quantities are not of the same kind. For example, joule per kelvin and J/K are

respectively the name and symbol of both a measurement unit of heat capacity and a measurement unit of entropy, which are generally not considered to be quantities of the same kind. However, in some cases special measurement unit terms are restricted to be used with quantities of a specific kind only. For example, the measurement unit ‘second to the power minus one’ (1/s) is termed hertz (Hz) when used for frequencies and becquerel (Bq) when used for activities of radionuclides.

Note 3: Measurement units of *quantities of dimension one* are numbers. In some cases these measurement units are given special terms, *e.g.*, radian, steradian, and decibel, or are expressed by quotients such as millimole per mole equal to 10^{-3} and microgram per kilogram equal to 10^{-9} .

Note 4: For a given quantity, the short term “unit” is often combined with the quantity term, such as “mass unit” or “unit of mass”.

Source: [VIM 1.9]. See also: Table 1.2.

1.55 nominal property

Property of a phenomenon, body, or substance, where the property has no magnitude.

Example 2: Colour of a paint sample.

Example 3: Colour of a spot test in chemistry.

Example 5: Sequence of amino acids in a polypeptide

Note 1: A nominal property has a value, which can be expressed in words, by alphanumerical codes, or by other means.

Note 2: ‘Nominal property value’ is not to be confused with *nominal quantity value*.

Note 3: A nominal property has no unit.

Source: [VIM 1.30] with Examples 1 and 4 omitted, and Note 3 added.

1.56 nominal quantity value

nominal value

Rounded or approximate *value* of a characterizing *quantity* of a *measuring instrument* or *measuring system* that provides guidance for its appropriate use

Example 1: 100 Ω as the nominal quantity value marked on a standard resistor.

Example 2: 1000 ml as the nominal quantity value marked on a single-mark volumetric flask.

Example 3: 0.1 mol/l as the nominal quantity value for amount-of-substance concentration of a solution of hydrogen chloride, HCl.

Example 4: $-20\text{ }^{\circ}\text{C}$ as a maximum Celsius temperature for storage.

Note: “Nominal quantity value” and “nominal value” should not be used for “nominal property value”.

Source: [VIM 4.6].

1.57 numerical quantity value

numerical value of a quantity

numerical value

Number in the expression of a *quantity value*, other than any number serving as the reference.

Note 1: For *quantities of dimension one*, the reference is a *measurement unit* which is a number and this is not considered as a part of the numerical quantity value.

Example: In an amount-of-substance fraction equal to 3 mmol/mol, the numerical quantity value is 3 and the unit is mmol/mol. The unit mmol/mol is numerically equal to 0.001, but this number 0.001 is not part of the numerical quantity value, which remains 3.

Note 2: For *quantities* that have a measurement unit (*i.e.* those other than *ordinal quantities*), the numerical value⁶ of a quantity Q is frequently denoted $\{Q\} = Q/[Q]$, where $[Q]$ denotes the measurement unit.

Example: For a quantity value of 5.7 kg, the numerical quantity value is $\{m\} = (5.7 \text{ kg})/\text{kg} = 5.7$. The same quantity value can be expressed as 5700 g in which case the numerical quantity value $\{m\} = (5700 \text{ g})/\text{g} = 5700$.

Source: [VIM 1.20].

1.58 ordinal quantity

Quantity, defined by a conventional *measurement procedure*, for which a total ordering relation can be established, according to magnitude, with other quantities of the same *kind of quantity*, but for which no algebraic operations among those quantities exist.

Example 1: Rockwell C hardness.

Example 2: Octane number for petroleum fuel.

Example 3: Earthquake strength on the Richter scale.

Example 4: Subjective level of abdominal pain on a scale from zero to five.

Note 1: Ordinal quantities can enter into empirical relations only and have neither *measurement units* nor *quantity dimensions*. Differences and ratios of ordinal quantities have no physical meaning.

Note 2: Ordinal quantities are arranged according to ordinal quantity-value scales [VIM 1.28].

Source: [VIM 1.26].

1.59 quantity

Property of a phenomenon, body, or substance, where the property has a magnitude that can be expressed as a number and a reference.

Note 1: The generic concept ‘quantity’ can be divided into several levels of specific concepts, as shown in Table 1.4. The left-hand side of the table shows specific concepts under ‘quantity’. These are generic concepts for the individual quantities in the right-hand column.

Note 2: A reference can be a *measurement unit*, a *measurement procedure*, a *reference material*, or a combination of such.

Note 3: Symbols for quantities are given in the ISO 80000³¹ series Quantities and units. The symbols for quantities are written in italics. A given symbol can indicate different quantities.

Note 4: The NPU format (Nomenclature for Properties and Units)⁵ preferred by IUPAC-IFCC for designations of quantities in laboratory medicine, is “System—Component; kind of quantity”, where each of the three segments may have parenthetical specifications.

Example: “Plasma(Blood)—Sodium ion; amount-of-substance concentration equal to 143 mmol/l in a given person at a given time”.

Note 5: A quantity as defined here is a scalar. However, a vector or a tensor, the components of which are quantities, is also considered to be a quantity.

Note 6: The concept ‘quantity’ may be generically divided into, e.g., ‘physical quantity’, ‘chemical quantity’, and ‘biological quantity’, or *base quantity* and *derived quantity*.

Source: [VIM 1.1] with amended Note 4.

Table 1.4 Concepts under ‘quantity’.

length, <i>l</i>	radius, <i>r</i> wavelength, λ	radius of circle <i>A</i> , r_A or $r(A)$ wavelength of the sodium D radiation, λ_D or $\lambda(D; \text{Na})$
energy, <i>E</i>	kinetic energy, <i>T</i> heat, <i>Q</i>	kinetic energy of particle <i>i</i> in a given system, T_i heat of vaporization of sample <i>i</i> of water, Q_i
electric charge, <i>Q</i>		electric charge of the proton, <i>e</i>
electric resistance, <i>R</i>		electric resistance of resistor <i>i</i> in a given circuit, R_i
amount-of-substance concentration of entity B, c_B		amount-of-substance concentration of ethanol in wine sample <i>i</i> , $c_i(\text{C}_2\text{H}_5\text{OH})$
number concentration of entity B, C_B		number concentration of erythrocytes in blood sample <i>i</i> , $C(\text{Erys}; B_i)$
Rockwell C hardness		Rockwell C hardness of steel sample <i>i</i> , HRC_i

1.60 quantity dimension

dimension of a quantity
dimension

Expression of the dependence of a *quantity* on the *base quantities* of a *system of quantities* as a product of powers of factors corresponding to the base quantities, omitting any numerical factor.

Example 1: In the *International System of Quantities* (ISQ), the quantity dimension of force F is denoted by $\dim F = \text{LMT}^{-2}$.

Example 2: In the same system of quantities, $\dim \gamma_B = \text{ML}^{-3}$ is the quantity dimension of mass concentration of *component* B, and ML^{-3} is also the quantity dimension of mass density (volumic mass), ρ .

Note 1: A power of a factor is the factor raised to an exponent. Each factor is the dimension of a base quantity.

Note 2: The conventional symbolic representation of the dimension of a base quantity is a single upper-case letter in roman (upright) sans-serif type. The conventional symbolic representation of the dimension of a *derived quantity* is the product of powers of the dimensions of the base quantities according to the definition of the derived quantity. The dimension of a quantity Q is denoted by $\dim Q$.

Note 3: In deriving the dimension of a quantity, no account is taken of its scalar, vector or tensor character.

Note 4: In a given system of quantities,
— quantities of the same *kind* have the same quantity dimension,
— quantities of different quantity dimensions are always of different kinds, and
— quantities having the same quantity dimension are not necessarily of the same kind.

Note 5: Symbols representing the dimensions of the base quantities in the ISQ are given in Table 1.5.

Source: [VIM 1.7] with Example 3 omitted.

1.61 quantity of dimension one

dimensionless quantity

Quantity for which all the exponents of the factors corresponding to the *base quantities* in its *quantity dimension* are zero.

Note 1: The term “dimensionless quantity” is commonly used and is kept here for historical reasons. It stems from the fact that all exponents are zero in the symbolic representation of the dimension for such quantities. The term “quantity of dimension one” reflects the convention in which the symbolic representation of the dimension for such quantities is the symbol 1 (see ref. 31).

Note 2: The *measurement units* and *values* of quantities of dimension one are numbers, but the quantities convey more information than a number.

Table 1.5 Symbols for dimensions of base quantities of the ISQ.

Base quantity	Symbol for dimension
length	L
mass	M
time	T
<i>electric current</i>	I
thermodynamic temperature	Θ
amount of substance	N
luminous intensity	J

Thus, the dimension of a quantity Q is denoted by $\dim Q = \text{L}^\alpha \text{M}^\beta \text{T}^\gamma \Theta^\delta \text{N}^\epsilon \text{J}^\eta$ where the exponents, termed dimensional exponents, are positive, negative, or zero.

Note 3: Some quantities of dimension one are defined as a ratio of two quantities of the same *kind*.

Examples: Plane angle, solid angle, refractive index, relative permeability, mass fraction, friction factor, Mach number.

Note 4: Numbers of entities are quantities of dimension one.

Examples: Number of turns in a coil, number of molecules in a given sample, degeneracy of the energy levels of a quantum system.

Source: [VIM 1.8].

1.62 quantity value

value of a quantity

value

Number and reference together expressing magnitude of a *quantity*.

Example 7: Rockwell C hardness of a given sample: 43.5 HRC.

Example 8: Mass fraction of cadmium in a given sample of copper alloy: 3 µg/kg or 3×10^{-9} .

Example 9: Molality of Pb^{2+} in a given sample of river water: 1.76 µmol/kg.

Example 10: Arbitrary amount-of-substance concentration of lutropin in a given sample of human blood plasma (WHO International Standard 80/552 used as a calibrator): 5.0 IU/l, where “IU” stands for “WHO International Unit”.

Note 1: According to the type of reference, a quantity value is either
— a product of a number and a *measurement unit* (see Example 9); the measurement unit one is generally not indicated for *quantities of dimension one*, (see Example 8), or
— a number and a reference to a *measurement procedure* (see Example 7), or
— a number and a *reference material* (see Example 10).

Source: [VIM 1.19] with Examples 1 to 6 and Notes 2 to 4 omitted, and with minor amendment to Example 8. See also: *true quantity value*.

1.63 reference quantity value

reference value

Quantity value used as a basis for comparison with values of *quantities* of the same *kind*.

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

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

- (a) a material, *e.g.*, a *certified reference material*,
- (b) a device, *e.g.*, a stabilized laser,
- (c) a *reference measurement procedure*, or
- (d) a comparison of *measurement standards*.

Source: [VIM 5.18].

1.64 system of quantities

Set of *quantities* together with a set of non-contradictory equations relating those quantities.

Note: *Ordinal quantities*, such as Rockwell C hardness, are usually not considered to be part of a system of quantities because they are related to other quantities through empirical relations only.

Source: [VIM 1.3].

1.65 system of units

Set of *base units* and *derived units*, together with their multiples and submultiples, defined in accordance with given rules, for a given *system of quantities*.

Source: [VIM 1.13].

1.66 true quantity value

true value of a quantity
true value

Quantity value consistent with the definition of a *quantity*.

Note 1: In the Error Approach to describing *measurement*, a true quantity value is considered unique and, in practice, unknowable. The Uncertainty Approach³⁴ is to recognize that, owing to the inherently incomplete amount of detail in the definition of a quantity, there is not a single true quantity value but rather a set of true quantity values consistent with the definition. However, this set of values is, in principle and in practice, unknowable. Other approaches dispense altogether with the concept of true quantity value and rely on the concept of *metrological compatibility of measurement results* for assessing their validity.

Note 2: In the special case of a fundamental physical constant,³⁵ the quantity is considered to have a single true quantity value.

Note 3: When the *definitional measurement uncertainty* associated with the *measurand* is considered to be negligible compared to the other components of the *measurement uncertainty*, the measurand may be considered to have an “essentially unique” true quantity value. This is the approach taken by the GUM³⁴ and associated documents, where the modifier “true” is considered to be redundant.

Source: [VIM 2.11].

1.67 unitary quantity

Quantity with a magnitude expressed as a reference quantity multiplied by a number.

Note: In the VIM,¹ the concept is denoted as “quantity expressed by a measurement unit” in the concept diagram Figure A.1 and is referred to as “quantities other than ordinal quantities”, e.g., in ref. 1 entry 1.21, and as “non-ordinal quantity” in Note 1 to ref. 1 entry 2.41.

See also: ref. 16 and 36.

1.5 Concepts on Measurement and Examination**1.68 critical value, L_c**

critical level
decision level

Measured quantity value for a *quantity* 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_α) is used for the concept ‘critical value’.³⁷

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’³⁸ of measurement procedures is *limit of detection*.

See also: ref. 39. Source: ref. 2 with added reference.

1.69 detector

Device or substance that indicates the presence of a phenomenon, body, or substance when a threshold value of an associated *quantity* is exceeded.

Examples: Halogen leak detector, litmus paper.

Note 1: In some fields, the term “detector” is used for the concept of *sensor*.

Note 2: In chemistry, the term “indicator” is frequently used for this concept.

Source: [VIM 3.9].

1.70 examination

Process of experimentally obtaining one or more nominal property values that can reasonably be attributed to a nominal property.

Source: ref. 13 entry 2.6 with Notes and Examples omitted.

1.71 examination uncertainty

Fraction of examined values that are different from a reference nominal property value among all the examined values provided.

Source: ref. 13 entry 3.9 with Notes and Examples omitted.

1.72 examination traceability

Property of an examination result whereby it can be related to a reference through a documented unbroken chain of examination calibrations, each contributing to the *examination uncertainty*.

Source: ref. 13 entry 3.21 with Note omitted.

Note: In ref. 13 entry 3.4 ‘examination result’ is defined as “set of nominal property values being attributed to an examinand together with any other available relevant information”.

1.73 examinand

See: *analyte*.

1.74 influence quantity

Quantity that, in a direct *measurement*, does not affect the quantity that is actually measured, but affects the relation between the *indication* and the *measurement result*.

Example 2: Amount-of-substance concentration of bilirubin in a direct measurement of haemoglobin amount-of-substance concentration in human blood plasma.

Example 4: Background pressure in the ion source of a mass spectrometer during a measurement of amount-of-substance fraction.

Note 1: An indirect measurement involves a combination of direct measurements, each of which may be affected by influence quantities.

Source: [VIM 2.52] with Examples 1 and 3 and Note 2 omitted.

1.75 input quantity in a measurement model

input quantity

Quantity that must be measured, or a quantity, the *value* of which can be otherwise obtained, in order to calculate a *measured quantity value* of a *measurand*.

Example: When the length of a steel rod at a specified temperature is the measurand, the actual temperature, the length at that actual temperature, and the linear thermal expansion coefficient of the rod are input quantities in a *measurement model*.

Note 1: An input quantity in a measurement model is often an output quantity of a *measuring system*.

Note 2: *Indications, corrections, and influence quantities* can be input quantities in a measurement model.

Source: [VIM 2.50]. See also: *measurement function*.

1.76 indication

Quantity value provided by a *measurement instrument* or a *measuring system*.

Note 1: An indication may be presented in visual or acoustic form or may be transferred to another device. An indication is often given by the position of a pointer on the display for analog outputs, a displayed or printed number for digital outputs, a code pattern for code outputs, or an assigned quantity value for *material measures*.

Note 2: An indication and a corresponding value of the *quantity* being measured are not necessarily values of quantities of the same *kind*.

Note 3: In many analytical instruments, the detector response is converted into an indication being linearly related to the value of the quantity to be measured. Compare *linearity of a measuring system*

Example: The indication provided by a spectrometer may be linearly related to the *radiant power* detected, or to *transmittance*, *absorbance* or *absorption coefficient* of a *sample*, or to the concentration of a specific analyte in the sample. See Chapter 6.

Source: [VIM 4.1] with added Note 3 with Example. See also: *property value assignment*.

1.77 measurand

Quantity intended to be measured.

Note 1: The specification of a measurand requires knowledge of the *kind of quantity*, 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* 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* is necessary.

Example 1: The electric potential difference between the terminals of a battery decreases 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.

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 may be applied.

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.

Note 5: The measurand may be operationally defined by reference to a documented *measurement procedure* to which only *quantity values* obtained by the same procedure can be compared.⁴⁰

Source: [VIM 2.3] with Note 2 omitted, minor clarification to Example 1, and added Note 5.

1.78 measured quantity value

measured value of a quantity

measured value

Quantity value representing a *measurement result*.

Note 1: For a *measurement* involving replicate *indications*, each indication can be used to provide a corresponding measured quantity value. This set of individual measured quantity values can be used to calculate a resulting measured quantity value, such as an average or median, usually with a decreased associated *measurement uncertainty*.

Note 2: When the range of the *true quantity values* believed to represent the *measurand* is small compared with the measurement uncertainty, a measured quantity value can be considered to be an estimate of an essentially unique *true quantity value* and is often an average or median of individual measured quantity values obtained through replicate measurements.

Note 3: In the case where the range of the true quantity values believed to represent the measurand is not small compared with the measurement uncertainty, a measured quantity value is often an estimate of an average or median of the set of true quantity values.

Note 4: In the GUM,³⁴ the terms “result of measurement” and “estimate of the value of the measurand” or just “estimate of the measurand” are used for ‘measured quantity value’.

Source: [VIM 2.10].

1.79 measurement

Process of experimentally obtaining one or more *quantity values* that can reasonably be attributed to a *quantity*.

Note 1: Measurement does not apply to *nominal properties*.

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*, a *measurement procedure*, and a calibrated *measuring system* operating according to the specified measurement procedure, including the measurement conditions.

Source: [VIM 2.1].

Note 4: Measurement is a subordinate concept of *determination* and so “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 *specified requirement* (i.e., in *conformity assessment*), measurement is often termed *testing*.

1.80 measurement function

Function of *quantities*, the value of which, when calculated using known *quantity values* for the *input quantities in a measurement model*, is a *measured quantity value* of the *output quantity in the measurement model*.

Note 1: If a *measurement model* $h(Y, X_1, \dots, X_n) = 0$ can explicitly be written as $Y = f(X_1, \dots, X_n)$, where Y is the output quantity in the measurement model, the function f is the measurement function. More generally, f may symbolize an algorithm, yielding for input quantity values x_1, \dots, x_n a corresponding unique output quantity value $y = f(x_1, \dots, x_n)$.

Note 2: A measurement function is also used to calculate the *measurement uncertainty* associated with the measured quantity value of Y .

Source: [VIM 2.49].

1.81 measurement method

method of measurement

Generic description of a logical organization of operations used in a *measurement*.

Note: Measurement methods may be qualified in various ways such as:

- substitution measurement method,
- differential measurement method, and
- null measurement method; or
- direct measurement method, and
- indirect measurement method. (See IEC 60050-300:2001⁴¹).

Source: [VIM 2.5].

1.82 measurement model

model of measurement
model

Mathematical relation among all *quantities* known to be involved in a *measurement*.

Note 1: A general form of a measurement model is the equation $h(Y, X_1, \dots, X_n) = 0$, where Y , the *output quantity in the measurement model*, is the *measurand*, the *quantity value* of which is to be inferred from information about *input quantities in the measurement model* X_1, \dots, X_n .

Note 2: In more complex cases where there are two or more output quantities in a measurement model, the measurement model consists of more than one equation.

Source: [VIM 2.48].

1.83 measurement principle

principle of measurement

Phenomenon serving as a basis of a *measurement*.

Example 1: Thermoelectric effect applied to the measurement of temperature.

Example 2: Energy absorption applied to the measurement of amount-of-substance concentration.

Example 3: Lowering of the concentration of glucose in blood in a fasting rabbit applied to the measurement of insulin concentration in a preparation.

Note: The phenomenon can be of a physical, chemical, or biological nature.

Source: [VIM 2.4].

1.84 measurement procedure

Detailed description of a *measurement* according to one or more *measurement principles* and to a given *measurement method*, based on a *measurement model* and including any calculation to obtain a *measurement result*.

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 78-2⁴² or Annex A of the Eurachem Guide “The Fitness for Purpose of Analytical Methods”.¹⁴

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

Note 6: ISO/IEC 17025⁴³ uses the term “method” for measurement procedure. “Examination procedure” is defined for medical laboratories.^{5,44}

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* and *bioassay*.

See also: *method performance study*.

1.85 measurement result

Set of *quantity values* being attributed to a *measurand* together with any other available relevant information.

Note 1: A measurement result generally contains “relevant information” about the set of quantity values, such that some may be more representative of the measurand than others. This may be expressed in the form of a probability density function (PDF).

Note 2: A measurement result is generally expressed as a single *measured quantity value* and a *measurement uncertainty*. If the measurement uncertainty is

considered to be negligible for some purpose, the measurement result may be expressed as a single measured quantity value. In many fields, this is the common way of expressing a *measurement result*.

Source: [VIM 2.9] with Note 3 omitted.

1.86 measuring instrument

Device used for making *measurements*, alone or in conjunction with one or more supplementary devices.

Note 1: A measuring instrument that can be used alone is a *measuring system*.

Source: [VIM 3.1] with Note 2 omitted.

1.87 measuring interval

See: *working interval*.

1.88 measuring system

Set of one or more *measuring instruments* and often other devices, including any reagent and supply, assembled and adapted to give information used to generate *measured quantity values* within specified intervals for *quantities* of specified *kinds*.

Note: A measuring system may consist of only one measuring instrument.

Source: [VIM 3.2].

1.89 metrology

Science of *measurement* and its application.

Note: Metrology includes all theoretical and practical aspects of measurement, whatever the *measurement uncertainty* and field of application.

Source: [VIM 2.2].

1.90 output quantity in a measurement model

output quantity

Quantity, the *measured value* of which is calculated using the *values* of *input quantities in a measurement model*.

Source: [VIM 2.51].

1.91 primary reference measurement procedure

primary reference procedure

Reference measurement procedure used to obtain a *measurement result* without relation to a *measurement standard* for a *quantity* of the same *kind*.

Example The volume of water delivered by a 50 ml pipette at 20 °C is measured by weighing the water delivered by the pipette into a beaker, taking the mass of beaker plus water minus the mass of the initially empty beaker, and correcting the mass difference for the actual water temperature using the volumic mass (mass density).

Note 1: The Consultative Committee for Amount of Substance – Metrology in Chemistry (CCQM) uses the term “primary method of measurement” for this concept.

Source: [VIM 2.8] with Note 2 omitted.

1.92 quantity calculus

algebra of quantities

Rules and operations of algebra applied to *unitary quantities*.

Note 1: In quantity calculus symbols are consistently used to represent *quantities* as a product of a *numerical quantity value* and a *measurement unit*, rather than their numerical values expressed in certain units.

Note 2: Algebraic relations between quantities, such as equations or functions, are independent of the choice of measurement units, and therefore preferred to expressions based on *numerical values*.

Note 3: VIM 1.21 defines quantity calculus as “set of mathematical rules and operations applied to quantities other than ordinal quantities”

Source: ref. 6 p. 3.

1.93 reference measurement procedure

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

Source: [VIM 2.7].

1.94 resolution

Smallest change in a *quantity* being measured that causes a perceptible change in the corresponding *indication*.

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

Note 2: When a *measuring instrument* or *measuring system* with digital indication is used, the minimum perceptible change equals the minimum difference between two indications. (See: “resolution of a displaying device”¹ entry 4.15).

Source: [VIM 4.14] with added Note 2.

1.95 response time of a measuring system

response time

Time difference between the initiation of a *measurement* and the attainment of an *indication* to obtain a *measurement result* meeting a *target measurement uncertainty*.

Source: ref. 45.

1.96 selectivity of a measuring system

selectivity

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

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

Example 4: *Capability* of a measuring system for ionizing radiation to respond to a given radiation to be measured in the presence of concomitant radiation.

Example 5: *Capability* of a measuring system to measure the amount-of-substance concentration of creatininium in blood plasma by a Jaffé procedure without being influenced by the glucose, urate, ketone, and protein concentrations. In *analytical chemistry* these latter substances are often termed as potential *interferents* and their influence is termed as *interference*.

Example 6: *Capability* of a mass spectrometer to measure the amount-of-substance abundance of the ²⁸Si isotope and of the ³⁰Si isotope in silicon from a geological deposit without influence between the two, or from the ²⁹Si isotope.

Note 2: In chemistry, the measured quantities often involve different *components* in the *system* undergoing *measurement* and these quantities are not necessarily of the same *kind*.

Note 3: In chemistry, selectivity of a measuring system is usually obtained for quantities with selected components in concentrations within stated intervals.

Source: [VIM 4.13] with Examples 2 and 3 omitted, an addition to Example 5 and Notes 1 and 4 omitted. See also *analytical selectivity*.

1.97 sensor

Element of a *measuring system* that is directly affected by a phenomenon, body, or substance carrying a *quantity* to be measured.

Examples: Sensing coil of a platinum resistance thermometer, rotor of a turbine flow meter, Bourdon tube of a pressure gauge, float of a level-measuring instrument, photocell of a spectrometer, thermotropic liquid crystal which changes colour as a function of temperature.

Note: In some fields, the term “detector” is used for this concept.

Source: [VIM 3.8].

1.98 stability of a measuring instrument

stability

Property of a *measuring instrument*, whereby its metrological properties remain constant in time.

Note 1: Stability may be quantified in several ways.

Example 1: In terms of the duration of a time interval over which a metrological property changes to a stated extent.

Example 2: In terms of the change of a property over a stated time interval.

Note 2: The term “stability” is also used for *material stability*.

Source: [VIM 4.19] with added Note 2.

1.99 testing

test

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

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

See also: ref. 46, *inspection*.

1.6 Concepts Related to Measurement Error and Measurement Uncertainty

It is vital to report a *measurement uncertainty* estimate along with a *measured quantity value*. In brief, a report of a *measurement result* should contain a statement about what the expected ‘best estimate’ for the *true value* is, as well as a statement of the probable interval of possible values specifying the uncertainty. The significant contributions to the uncertainty from all relevant sources should be estimated as parts of an *uncertainty budget*. The mechanisms for assessing uncertainty are given in detail by JCGM 100:2008 (GUM).³⁴ The Eurachem/CITAC Guide CG4⁴⁷ is recommended as a particular source of information for chemists.

1.100 accuracy class

Class of *measuring instruments* or *measuring systems* that meet stated metrological requirements that are intended to keep *measurement errors* or *instrumental measurement uncertainties* within specified limits under specified operating conditions.

Note 1: An accuracy class is usually denoted by a number or symbol adopted by convention.

Note 2: Accuracy class applies to *material measures*.

Source: [VIM 4.25].

1.101 combined standard measurement uncertainty

combined standard uncertainty

Standard measurement uncertainty that is obtained using the individual standard measurement uncertainties associated with the *input quantities in a measurement model*.

Note: In case of correlations of input quantities in a measurement model, covariances must also be taken into account when calculating the combined standard measurement uncertainty; see also ref. 34 2.3.4.

Source: [VIM 2.31].

1.102 correction

Compensation for an estimated *systematic effect*.

Note 2: The compensation can take different forms, such as an addend or a factor, or can be deduced from a table.

Source: [VIM 2.53] with Note 1 omitted.

1.103 coverage factor

Number larger than one by which a *combined standard measurement uncertainty* is multiplied to obtain an *expanded measurement uncertainty*.

Note: A coverage factor is usually symbolized k (see ref. 34 2.3.6)

Source: [VIM 2.38].

1.104 coverage interval

Interval containing the set of *true quantity values* of a *measurand* with a stated probability, based on the information available.

Note 1: A coverage interval does not need to be centred on the chosen *measured quantity value* (see ref. 48).

Note 2: A coverage interval should not be termed “confidence interval” to avoid confusion with the statistical concept (see ref. 34 clause 6.2.2).

Note 3: A coverage interval can be derived from an *expanded measurement uncertainty* (see ref. 34 clause 2.3.5).

Source: [VIM 2.36].

1.105 coverage probability

Probability that the set of *true quantity values* of a *measurand* is contained within a specified *coverage interval*.

Note 1: This definition pertains to the uncertainty approach as presented in the GUM.³⁴

Note 2: The coverage probability is also termed “level of confidence” in the GUM.³⁴

Source: [VIM 2.37].

1.106 definitional measurement uncertainty

Component of *measurement uncertainty* resulting from the finite extent of detail in the definition of a *measurand*.

Note 1: Definitional uncertainty is the practical minimum measurement uncertainty achievable in any *measurement* of a given measurand.

Note 2: Any change in the descriptive detail leads to another definitional uncertainty.

Note 3: In the GUM³⁴ D.3.4 and in IEC 60359⁴⁹ the concept ‘definitional uncertainty’ is termed “intrinsic uncertainty”.

Source: [VIM 2.27].

1.107 drift of a measuring system

See: *instrumental drift*.

1.108 expanded measurement uncertainty

expanded uncertainty

Product of a *combined standard measurement uncertainty* and a factor larger than the number one.

Note 1: The factor depends upon the type of probability distribution of the *output quantity in a measurement model* and on the selected *coverage probability*.

Note 2: The term “factor” in this definition refers to a *coverage factor*.

Source: [VIM 2.35] with Note 3 omitted.

1.109 instrumental biasAverage of replicate *indications* minus a *reference quantity value*.

Source: [VIM 4.20].

1.110 instrumental drift

drift

Continuous or incremental change over time in *indication*, due to changes in metrological properties of a *measuring instrument*.

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

Note 2: The definition of instrumental drift may also apply to changes in indication due to changes in metrological properties of a *measuring system*, when it is termed “drift of a measuring system”.

Source: [VIM 4.21] with added Note.

1.111 instrumental measurement uncertaintyComponent of *measurement uncertainty* arising from a *measuring instrument* or *measuring system* in use.

Note 1: Instrumental measurement uncertainty is obtained through *calibration* of a measuring instrument or measuring system, except for a *primary measurement standard* for which other means are used.

Note 2: Instrumental measurement uncertainty is used in a *Type B evaluation of measurement uncertainty*.

Note 3: Information relevant to instrumental measurement uncertainty may be given in the instrument specifications.

Source: [VIM 4.24].

1.112 intermediate measurement precision

intermediate precision

Measurement precision under a set of *intermediate precision conditions of measurement*.

Note: “Intralaboratory precision”, “within-laboratory reproducibility”, or “within-laboratory precision” is sometimes used as a synonym of intermediate measurement precision.

Source: ref. 2 entry 3.31 with amendment to Note. Definition is [VIM 2.23].

1.113 intermediate precision condition of measurement

intermediate precision condition

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

Note 1: The changes can include new *calibrations*, *calibrators*, operators, and *measuring systems*.

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

Source: [VIM 2.22] with Note 3 omitted.

1.114 laboratory bias

Contribution to *measurement bias* that is attributed to *systematic effects* on *measurement results* made in a laboratory.

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

1.115 level of confidence

See: *coverage probability*.

1.116 limit of detection, (LOD)

detection limit, (DL)

True quantity value for a *quantity* 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 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* Note 2) of 95 % for a statistical test for non-zero true value of the quantity of the component, 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* 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, $1 - \text{error probability}$, to the conclusion that the system is not in the basic state”.²⁶

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 legislations ‘detection capability’ (denoted as $\text{CC}\beta$) 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 ”.³⁷

Note 11: The ISO 11843 series “Capability of detection” covers a wide field related 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.³⁸

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”.⁵⁰

See also: ref. 39, 51 and 52.

1.117 limit of quantification, (LOQ)

quantification limit

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

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

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

Note 3: The smallest and largest measured quantity values 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 the LLOQ can be compared.

See also: ref. 39 and 53.

1.118 linear interval

linear range

See: *linearity of a measuring system*.

1.119 linearity of a measuring system

linearity

Ability of a *measuring system* to provide *measured quantity values* that are directly proportional to the *quantity value* of the *measurand*.

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*.

See also: ref. 54.

1.120 maximum permissible measurement error, (MPE)

maximum permissible error

limit of error

Extreme value of *measurement error*, with respect to a known *reference quantity value*, permitted by specifications or regulations for a given *measurement, measurement instrument, or measuring system*.

Note 1: Usually, the term “maximum permissible errors” or “limits of error” is used where there are two extreme values.

Note 2: The term “tolerance” should not be used to designate ‘maximum permissible error’.

Source: [VIM 4.26] with added initialism.

1.121 measurement accuracy

accuracy of measurement

accuracy

Closeness of agreement between a *measured quantity value* and a *true quantity value* of a *measurand*.

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

Note 2: The term “measurement accuracy” should not be used for *measurement trueness* and the term “measurement precision” should not be used for ‘measurement accuracy’, which, however, is related to both these concepts.

Note 3: ‘Measurement accuracy’ is sometimes understood as closeness of agreement between measured quantity values that are being attributed to the measurand.

Source: [VIM 2.13].

1.122 measurement bias

bias

Estimate of a *systematic measurement error*.

Source: [VIM 2.18].

1.123 measurement error

error of measurement

error

Measured quantity value minus a *reference quantity value*.

Note 1: The concept of ‘measurement error’ can be used both

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

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

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

Source: [VIM 2.16].

1.124 measurement precision

precision

Closeness of agreement between *indications* or *measured quantity values* obtained by replicate *measurements* on the same or similar objects under specified conditions.

Note 1 Measurement precision is usually expressed numerically by measures of imprecision, such as standard deviation, variance, or coefficient of variation under the specified conditions of measurement.

Note 2: The ‘specified conditions’ can be, for example, *repeatability conditions of measurement*, intermediate precision conditions of measurement, or *reproducibility conditions of measurement* (see ref. 55).

Note 3: Measurement precision is used to define *measurement repeatability*, *intermediate measurement precision*, and *measurement reproducibility*.

Note 4: Sometimes “measurement precision” is erroneously used to mean *measurement accuracy*.

Source: [VIM 2.15].

1.125 measurement procedure bias

measurement method bias

Contribution to *measurement bias* that is attributed to *systematic effects* on *measurement results* made according to a *measurement procedure*.

Note 1: Measurement procedure bias covers *instrumental bias*.

Note 2: Contributions to measurement procedure bias are calculated during *procedure validation*.¹⁴

Note 3: Measurement bias in *analytical chemistry* may be considered to include *run bias*, *laboratory bias*, and measurement procedure bias.⁵⁶

1.126 measurement repeatability

repeatability

Measurement precision under a set of *repeatability conditions of measurement*.

Source: [VIM 2.21].

1.127 measurement reproducibility

reproducibility

Measurement precision under *reproducibility conditions of measurement*.

Note 1: Relevant statistical terms are given in ISO 5725-1⁵⁷ and ISO 5725-2.⁵⁸

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

Source: [VIM 2.25] with added Note 2.

1.128 measurement trueness

trueness of measurement

trueness

Closeness of agreement between the average of an infinite number of replicate *measured quantity values* and a *reference quantity value*.

Note 1: Measurement trueness is not a *quantity* and thus cannot be expressed numerically, but measures for closeness of agreement are given in ISO 5725.⁵⁵

Note 2: Measurement trueness is inversely related to *systematic measurement error*, but is not related to *random measurement error*.

Note 3: “Measurement accuracy” should not be used for ‘measurement trueness’.

Source: [VIM 2.14].

1.129 measurement uncertainty

uncertainty of measurement

uncertainty

Non-negative parameter characterizing the dispersion of the *quantity values* being attributed to a *measurand*, based on the information used.

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

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

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

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

Source: [VIM 2.26]. For Note 1 see *property value assignment, conventional quantity value*
Note 4.

1.130 random measurement error

random error of measurement
random error

Component of *measurement error* that in replicate *measurements* varies in an unpredictable manner.

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

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

Note 3: Random measurement error equals measurement error minus *systematic measurement error*.

Source: [VIM 2.19].

1.131 relative standard measurement uncertainty

Standard measurement uncertainty divided by the absolute value of the *measured quantity value*.

Source: [VIM 2.32].

1.132 repeatability condition of measurement

repeatability condition

Condition of *measurement*, out of a set of conditions that includes the same *measurement procedure*, same operators, same *measuring system*, same operating conditions, 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.

Note 2: In ISO 3534-2, “same operator” (singular) is stipulated as a repeatability condition. The VIM request of “same operators” (plural) should be understood such that if two or more operators contribute to one measurement, they should be involved in the same way in repeated measurements.²⁶

Note 3: In *analytical chemistry*, the phrase “under repeatability conditions” refers to the above specified set of conditions.

Note 4: A set of measurements under repeatability conditions is often termed *analytical run*.

Source: [VIM 2.20] with Note 2 replaced and Notes 3 and 4 added.

1.133 reproducibility condition of measurement

reproducibility condition

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

Note 1: The different measuring systems may use different *measurement procedures*.

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

Source: [VIM 2.24].

1.134 run bias

Contribution to *measurement bias* that is attributed to *systematic effects* on *measurement results* 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*.

1.135 standard measurement uncertainty

standard uncertainty of measurement

standard uncertainty

Measurement uncertainty expressed as a standard deviation.

Source: [VIM 2.30].

1.136 systematic effect

Recognized effect of an *influence quantity* on a *measured quantity value*.

Note: A systematic effect can be compensated for by a *correction*.

1.137 systematic measurement error

systematic error of measurement

systematic error

Component of *measurement error* that in replicate *measurements* remains constant or varies in a predictable manner.

Note 1: A *reference quantity value* for a systematic measurement error is a *true quantity value*, or a *measured quantity value* of a *measurement standard* of negligible *measurement uncertainty*, or a *conventional quantity value*.

Note 2: Systematic measurement error, and its causes, can be known or unknown. A *correction* can be applied to compensate for a known systematic measurement error.

Note 3: Systematic measurement error equals measurement error minus *random measurement error*.

Source: [VIM 2.17].

1.138 Type A evaluation of measurement uncertainty

Type A evaluation

Evaluation of a component of *measurement uncertainty* by a statistical analysis of *measured quantity values* obtained under defined measurement conditions.

Note 1: For various types of measurement conditions, see *repeatability condition of measurement*, *intermediate precision condition of measurement*, and *reproducibility condition of measurement*.

See also: ref. 34 entry 2.3.2. Source: [VIM 2.28] with Notes 2 and 3 omitted.

1.139 Type B evaluation of measurement uncertainty

Type B evaluation

Evaluation of a component of *measurement uncertainty* determined by means other than a *Type A evaluation of measurement uncertainty*.

Examples: Evaluation based on information

- associated with authoritative published *quantity values*,
- associated with the quantity value of a *certified reference material*,
- obtained from a *calibration certificate*,
- about *drift*,
- obtained from the *accuracy class* of a verified *measuring instrument*, and
- obtained from limits deduced through personal experience.

Note: See also GUM,³⁴ 2.3.3.

Source: [VIM 2.29].

1.140 uncertainty budget

Statement of a *measurement uncertainty*, of the components of that measurement uncertainty, and of their calculation and combination.

Note: An uncertainty budget should include the *measurement model*, estimates, and measurement uncertainties, associated with the *quantities* in the measurement model, covariances, type of applied probability density functions, degrees of freedom, type of evaluation of measurement uncertainty, and any *coverage factor*.

Source: [VIM 2.33].

1.7 Concepts Related to Calibration

Almost every *measurement* in *analytical chemistry* is calibrated in the two-step process described by the definition below (see *calibration*). To assure *metrological traceability* the *quantity values* of the *measurement standards* must themselves be traceable.⁵⁹ Use of a *certified reference material* ensures this if balances and volumetric equipment used to make up standards presented to the *measuring system* are also properly calibrated. *Measurement uncertainties* of quantity values of standards contribute to the overall *measurement uncertainty budget* for the *measurement result*. Traditionally, the relation between values provided by standards and corresponding *indications* is considered to be first order linear, and was constructed as a straight line graph. Now, with modern computing, quadratic, hyperbolic, and other forms are easily fitted to calibration data with measurement uncertainty, taking account of correlations if present.⁶⁰ *Classical least squares regression* tends to be the method of choice for constructing *calibration curves*, (See Chapter 2) but it must be understood that this assumes that the model is correct, with only Gaussian, homoscedastic, *random error* in the indications (none in the values of standards). If these conditions are not applicable to the calibration, then other kinds of fitting (e.g., *weighted least squares regression*, *errors in variables regression*) should be used. In *procedure validation* and *procedure verification* the range of values of the measurand for which the *calibration function* is valid is assessed (see Section 13.3). For terms relating to *reference materials* see Section 13.4.

1.141 analytical function

See: *calibration function*.

1.142 analytical sensitivity

See: *sensitivity of a measuring system*.

1.143 calibration

Operation that, under specified conditions, in a first step, establishes a relation between the *quantity values* with *measurement uncertainties* provided by *measurement standards* and corresponding *indications* with associated measurement

uncertainties and, in a second step, uses this information to establish a relation for obtaining a *measurement result* from an indication.

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

Note 2: Calibration should not be confused with adjustment of a measuring system, often mistakenly termed “self-calibration”, nor with *verification* of calibration.

Note 3: Often, the first step alone in the above definition is perceived as being calibration.

Source: [VIM 2.39].

1.144 calibration certificate

Document issued by a technically competent *organization* providing information about a *calibration*.

Note 1: The document may include a statement describing the calibration procedure and the *calibrators* (calibrants) applied along with the *calibration function*, *calibration curve* 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 17025.⁴³

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

Source: ref. 2 entry 3.17 with amendment to Note 1.

1.145 calibration curve

Expression of the relation between *indication* and corresponding *measured quantity value*.

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

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’ (see ref. 1 entry 4.30) is defined as a “Graphical expression of the relation between indication and corresponding measurement result”. A calibration diagram allows *instrumental measurement uncertainty* to be represented in it and so differs from a calibration curve. In *analytical chemistry* the distinction between calibration curve and calibration diagram is rarely made.

Source: [VIM 4.31] with added Notes 2, 3 and 4.

1.146 calibration function

Presentation of a *calibration curve* by a mathematical function.

Note 1: The calibration function is established by fitting the data from the first step of *calibration* using the *measured quantity values* provided by *measurement standards* as input variables to calculate the expected indication. A calibration function bears no information about *measurement uncertainty*. (See also Note 1 to *linearity of calibration* and 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* 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.

1.147 calibration hierarchy

Sequence of *calibrations* from a reference to the final *measuring system*, where the outcome of each calibration depends on the outcome of the previous calibration.

Note 1: *Measurement uncertainty* necessarily increases along the sequence of calibrations.

Note 2: The elements of a calibration hierarchy are one or more *measurement standards* and measuring systems operated according to *measurement procedures*.

Note 3: For this definition, the ‘reference’ can be a definition of a *measurement unit*, through its practical realization, or a measurement procedure, or a measurement standard.

Note 4: A comparison between two measurement standards may be viewed as a calibration if the comparison is used to check and, if necessary, correct the *quantity value* and measurement uncertainty attributed to one of the measurement standards.

Source: [VIM 2.40].

1.148 calibrator

Measurement standard used in calibration.

Note 1: The term “calibrator” is only used in certain fields.

Note 2: ISO Guide 30 gives the term “calibrant”.³

Source: [VIM 5.12] with added Note 2.

1.149 linearity of calibration

calibration linearity

Closeness of agreement between *indications* obtained using *calibrators* in the first step of a *calibration* and indications predicted by the *calibration function* for the calibrators’ *reference quantity values*.

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 calibration*), obtained by regression of calibration data or assessed from a residual plot. See also: ref. 61.

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: ref. 14.

1.150 measurement procedure with standard addition

standard addition

Measurement procedure in which *indications* are obtained for an *analytical sample* as well as for analytical samples with serial addition(s) of aliquots of a *measurement standard*.

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

Note 2: If the relation between the indications (*y*) and the quantities added (*x*) is obtained by linear regression of *y* on *x*, then the quantity in the analytical sample is $x_0 = b_0/b_1$ where $y = b_0 + b_1x$, *i.e.* the intercept divided by

the slope of a *calibration curve*. The *standard uncertainty* of the estimate x_0 , is

$$s_e(x_0) = \frac{s_{y/x}}{|b_1|} \sqrt{\frac{1}{n} + \frac{\bar{y}^2}{b_1^2 \sum_{i=1}^n (x_i - \bar{x})^2}}$$

where $s_{y/x}$ is the standard error of the regression, n the number of additions, and \bar{x} and \bar{y} the means of the x_i and y_i respectively. (See ref. 62 p. 8 and p. 157).

See also: ref. 9. Source: ref. 2 entry 3.50 with added Note 2.

1.151 measurement standard

etalon

Realization of the definition of a given *quantity*, with stated *quantity value* and associated *measurement uncertainty*, used as a reference.

Example 1: 1 kg mass measurement standard with an associated *standard measurement uncertainty* of 3 μg .

Example 2: 100 Ω measurement standard resistor with an associated standard measurement uncertainty of 1 $\mu\Omega$.

Example 3: Caesium *frequency* standard with a *relative standard measurement uncertainty* of 2×10^{-15} .

Example 4: Standard buffer solution with a pH of 7.072 with an associated standard measurement uncertainty of 0.006.

Example 5: Set of reference solutions of cortisol in human serum having a certified quantity value with measurement uncertainty for each solution.

Example 6: *Reference material* providing quantity values with measurement uncertainties for the mass concentration of each of ten different proteins.

Note 1: A ‘realization of the definition of a given quantity’ can be provided by a *measuring system*, a *material measure*, or a reference material.

Note 2: A measurement standard is frequently used as a reference in establishing *measured quantity values* and associated measurement uncertainties for other quantities of the same *kind*, thereby establishing *metrological traceability* through *calibration* of other measurement standards, *measuring instruments*, or measuring systems.

Note 3: The term “realization” is used here in the most general meaning. It denotes three procedures of “realization”. The first one consists in the physical realization of the *measurement unit* from its definition and is realization in the strictest sense. The second, termed “reproduction”, consists not in realizing the measurement unit from its definition, but in setting up a highly reproducible measurement standard based on a physical phenomenon, as it happens, *e.g.*, in case of use of frequency-stabilized lasers to establish a measurement standard for the metre, of the Josephson effect for the volt, or of the quantum Hall effect for the ohm. The third procedure consists in adopting a material measure as a measurement standard. It occurs in the case of the measurement standard of 1 kg.

Note 4: A standard measurement uncertainty associated with a measurement standard is always a component of the *combined standard measurement uncertainty* (see ref. 34 entry 2.3.4) in a *measurement result* obtained using the measurement standard. Frequently, this component is small compared with other components to the combined standard measurement uncertainty.

Note 5: Quantity value and measurement uncertainty must be determined at the time when the measurement standard is used.

Note 6: Several quantities of the same kind or of different kinds may be realized in one device which is commonly also termed a measurement standard.

Note 7: A measurement standard can be used as *internal standard* or as external standard.

Source: [VIM 5.1] with Note 7 replaced and Note 8 omitted.

1.152 metrological comparability of measurement results

metrological comparability

Comparability of *measurement results*, for *quantities* of a given *kind*, that are metrologically traceable to the same reference.

Example: Measurement results, for the distances between the Earth and the Moon, and between Paris and London, are metrologically comparable when they are both metrologically traceable to the same *measurement unit*, for instance the metre.

Note 1: See Note 1 to *metrological traceability*.

Note 2: Metrological comparability of measurement results does not necessitate that the *measured quantity values* and associated *measurement uncertainties* compared be of the same order of magnitude.

Source: [VIM 2.46].

1.153 metrological compatibility of measurement results

metrological compatibility

Property of a set of *measurement results* for a specified *measurand*, such that the absolute value of the difference of any pair of *measured quantity values* from two different measurement results is smaller than some chosen multiple of the *standard measurement uncertainty* 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* was assessed as being too small) or the measured *quantity* 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 square sum of their standard measurement uncertainties, while it is lower for positive covariance or higher for negative covariance.

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*, the concept ‘degree of equivalence’ is applied in special *interlaboratory comparisons* termed “key comparisons”. The degree of equivalence of each national standard is expressed quantitatively by two terms: its deviation from the key comparison reference value and the uncertainty of this deviation (at a *coverage probability* of approximately 95 %).⁶³ See also: *metrological equivalence of measurement results*.

Source: [VIM 2.47] with corrected Note 2 and added Note 3.

1.154 metrological equivalence of measurement results

equivalence of measurement results

Property of two or more *measurement results* for a given *measurand* which 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. See also: ref. 59.

1.155 metrological traceability

Property of a *measurement result* whereby the result can be related to a reference through a documented unbroken chain of *calibrations*, each contributing to the *measurement uncertainty*.

Note 1: For this definition, a 'reference' can be a definition of a *measurement unit* through its practical realization, or a *measurement procedure* including the measurement unit for a *unitary quantity*, or a *measurement standard*.

Note 2: Metrological traceability requires an established *calibration hierarchy*.

Note 3: Specification of the reference must include the time at which this reference was used in establishing the calibration hierarchy, along with any other relevant metrological information about the reference, such as when the first calibration in the calibration hierarchy was performed.

Note 4: For *measurements* with more than one *input quantity in the measurement model*, each of the input *quantity values* should itself be metrologically traceable and the calibration hierarchy involved may form a branched structure or a network. The effort involved in establishing metrological traceability for each input quantity value should be commensurate with its relative contribution to the measurement result.

Note 5: Metrological traceability of a measurement result does not ensure that the measurement uncertainty is adequate for a given purpose or that there is an absence of mistakes.

Note 6: A comparison between two measurement standards may be viewed as a calibration if the comparison is used to check and, if necessary, correct the quantity value and measurement uncertainty attributed to one of the measurement standards.

Note 7: The ILAC considers the elements for confirming metrological traceability to be an unbroken *metrological traceability chain* to an international *measurement standard* or a national measurement standard, a documented measurement uncertainty, a documented *measurement procedure*, accredited technical competence, metrological traceability to the *International System of Units*, and *calibration intervals*.⁶⁴

Note 8: The abbreviated term "traceability" is sometimes used to mean 'metrological traceability' as well as other concepts, such as 'sample traceability' or 'document traceability' or 'instrument traceability' or 'material traceability', where the history ("trace") of an item is meant. Therefore, the full term of "metrological traceability" is preferred if there is any risk of confusion.

Source: [VIM 2.41]. See also: *object traceability*.

1.156 metrological traceability chain

traceability chain

Sequence of *measurement standards* and *calibrations* that is used to relate a *measurement result* to a reference.

Note 1: A metrological traceability chain is defined through a *calibration hierarchy*.

Note 2: A metrological traceability chain is used to establish *metrological traceability* of a measurement result.

Note 3: A comparison between two measurement standards may be viewed as a calibration if the comparison is used to check and, if necessary, correct the *quantity value* and *measurement uncertainty* attributed to one of the measurement standards.

Source: [VIM 2.42].

1.157 **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.

See also: ref. 3 entry 2.1.8.

1.158 **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 ISO 9000¹⁷ (entry 3.6.13) the term defined is traceability. However, because of the potential confusion with *metrological traceability* it is recommended to use the full term if there is ambiguity.

1.159 **sensitivity of a measuring system**

sensitivity

Quotient of the change in an *indication* of a *measuring system* and the corresponding change in a *value* of a *quantity* being measured.

Note 1: 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*. (Definition and Notes 1 and 2 are [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*.

Note 6: In *analytical chemistry* sensitivity may be termed “analytical sensitivity”.

See also: ref. 14 Section 6.4. Source: ref. 2 entry 4.156 with added Note 6.

1.160 **working interval**

working range

Set of *quantity values* over which a *measuring instrument* or *measuring system* provides results with acceptable *measurement uncertainty*, under defined conditions.

Note 1: In some fields, the term is “measurement range”. In entry 4.7 of VIM, a similar concept termed “measuring interval” is defined.

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: ref. 14 Section 6.3. See also: *linearity of a measuring system* Note 2.

1.8 Terms, Symbols, Definitions and SI Units of Quantities and Constants

The compilation below is based on the IUPAC Green Book,⁶ IUPAC-IFCC Silver Book,⁵ ISO 80000-4 and ISO 80000-8.³¹ Symbols of *quantity* given here are recommendations; if different symbols are used, they should be clearly defined. Symbols for *base units* as quoted in Table 1.2 of *International System of Units* are mandatory.

The symbol for a quantity should be a single letter; capital and lower-case letters may both be used. The letter should be printed in italic type (tilted, sloping). When necessary, the symbol may be modified by subscripts and superscripts of specified meaning. These are printed in roman type (upright) except if they are themselves symbols for quantity. Conventionally, there are a few exceptions from the single-letter rule, most importantly pH and any pX (which, as a further exception, ‘p’ is printed in upright type). As a positive side-effect, the use of single-letter symbols simplifies the notation of products by waiving the need of giving multiplication operators explicitly.

Apart from answering the question “how much material?” by measuring one of the extensive quantities of the material (often mass or volume), a central task in *analytical chemistry* is to provide information on the quantitative composition of a *chemical substance*. A so called ‘compositional quantity’ relates an extensive quantity of a specified *component* to an extensive quantity of the material as a whole and in this way provides an intensive quantity of the material system, *i.e.*, one which is independent of its extent.

1.8.1 Quantities Answering the Question “How Much Material?”

To answer the question a *quantity* must be additive for independent, noninteracting subsystems. These quantities are termed “extensive quantities” out of which amount of substance, mass, and volume are used frequently in analytical practice. Table 1.6 gives such quantities at the macroscopic and atomic scales, and constants associated with them.

1.8.2 Quantities Describing the Composition of a Material

The quantitative composition of a material can be described with *quantities* relating an extensive quantity of a specified *component* (entity/species) to the same or another kind of extensive quantity of the material as a whole. The quotient of the two quantities is independent of the extend of the system why the resulting “compositional quantity” is termed “intensive” (see Section 1.8.4). In laboratory practice the multitude of compositional quantities is typically clustered according to the quantity of the *system* and termed respectively: compositional quantities based on the volume of the system are termed “concentration”, those related to the mass of the system are termed “content”; other clusters are related to amount of substance or number of entities.⁶⁶ Full account of the particular kind of compositional quantity under consideration is given specifying also the extensive quantity of the component, leading to *e.g.*, mass concentration or amount-of-substance content. The clusters must be distinguished from each other because for instance a mass fraction is not a mass concentration (see Table 1.7). The terms “concentration” or “content” should be used alone only if there is no risk of confusion.

Table 1.6 Quantities to specify “how much?”.

Quantity or constant	Symbol	Definition (relating to specified component B)	SI unit	Note
number of entities	N		1	1
amount of substance, chemical amount	n	$n_B = N_B/N_A$	mol	
Avogadro constant $N_A = 6.02214076 \times 10^{23} \text{ mol}^{-1}$	N_A	N/n	mol^{-1}	2
mass	m		kg	
molar mass	M	$M_B = m/n_B$	kg mol^{-1}	
length, distance	l, d, r		m	3
area	A		m^2	
volume	V		$\text{m}^3, \text{l (L)}$	4
atomic mass constant	m_u	$m_u = m_a(^{12}\text{C})/12$	kg	
unified atomic mass unit,	u	$u = m_a(^{12}\text{C})/12$	kg	4
dalton	Da	$\text{Da} = m_a(^{12}\text{C})/12$	kg	4
atomic mass, mass of atom	m_a		kg	
relative atomic mass (historically: atomic weight)	A_r	$A_r = m_a/m_u$	1	
standard atomic weight ⁶⁵ of element E	$A_r^\circ(\text{E})$		1	
atomic weight ⁶⁵ of an element E in a specific substance P	$A_r(\text{E}, \text{P})$		1	
mass of entity (molecule, formula unit)	m_f		kg	5
relative molecular mass (historically: molecular weight)	M_r	$M_r = m_f/m_u$	1	
charge number of ion B	z_B	$z_B = Q_B/e$	1	

1. Typical entities are atoms, molecules, ions, and particles, such as microbiological colony forming units (CFU).

2. The fixed constants defining the *SI* are given in Table 1.9 of Section 1.8.5. They do not carry any *measurement uncertainty*.

3. The Ångström $\text{Å} = 10^{-10} \text{ m}$ is widely used but is not an SI unit.

4. The litre, symbol “L” or “l”, the dalton, symbol “Da”, the unified atomic mass unit, symbol “u”, are non-SI units accepted for use with the SI. Dalton may be combined with the SI prefixes given in Table 1.3.

5. Formula unit denotes an entity specified as a group of atoms. Note that ‘formula unit’ is not a unit.

Table 1.7 Compositional quantities.

Quantity	Symbol	Definition (relating to specified component B, C)	SI unit	Note
amount-of-substance concentration, amount concentration, concentration	$c, [\text{B}]$	$c_B = n_B/V$	mol m^{-3}	1, 2
mass concentration	γ	$\gamma_B = m_B/V$	kg m^{-3}	1, 3
number concentration, number density	C	$C_B = N_B/V$	$1 \text{ m}^{-3} = \text{m}^{-3}$	1, 3
volume concentration	σ	$\sigma_B = V_B/V$	$\text{m}^3 \text{ m}^{-3} = 1$	1, 3
volume fraction	φ	$\varphi_B = V_B/\sum V_i$	$\text{m}^3 \text{ m}^{-3} = 1$	3, 4, 5
density, mass density	ρ	$\rho = m/V$	kg m^{-3}	6
mass content	v	$v_B = m_B/m$	$\text{kg kg}^{-1} = 1$	5, 7
mass fraction	w	$w_B = m_B/\sum m_i$	$\text{kg kg}^{-1} = 1$	5, 7
volume content	k	$k_B = V_B/m$	$\text{m}^3 \text{ kg}^{-1}$	7
amount-of-substance content, amount content	κ	$\kappa_B = n_B/m$	mol kg^{-1}	7
number content	K	$K_B = N_B/m$	$1 \text{ kg}^{-1} = \text{kg}^{-1}$	7
molality (of component B in solvent S)	b	$b_B = n_B/m_S$	mol kg^{-1}	8
amount-of-substance fraction, amount fraction, mole fraction	x	$x_B = n_B/\sum n_i$	$\text{mol mol}^{-1} = 1$	7

Table 1.7 (Continued)

Quantity	Symbol	Definition (relating to specified component B, C)	SI unit	Note
number fraction	X	$X_B = N_B/\sum N_i$	$1 \text{ } 1^{-1} = 1$	7
volume ratio	φ	$\varphi(B, C) = V_B/V_C$	$\text{m}^3 \text{ m}^{-3} = 1$	9
mass ratio	ζ	$\zeta(B, C) = m_B/m_C$	$\text{kg kg}^{-1} = 1$	9
amount-of-substance ratio, amount ratio, mole ratio	r	$r(B, C) = n_B/n_C$	$\text{mol mol}^{-1} = 1$	9

1. V is the volume of the system, in the case after mixing components.
2. The Chemistry and Human Health Division (VII) of IUPAC recommends that amount-of-substance concentration be abbreviated to "substance concentration".^{5,67}
3. Further quantities that describe compositions of mixtures can be found in ref. 66. See also ISO 80000.³¹ The terms should not be used without clarifying the definition.
4. For mixtures, V_i are the volumes of the components i prior to mixing.
5. With respect to the analysis of a given system, the summation of the mass (volume) Q_i refers to a set of non-overlapping components i covering the entire system so that $\sum Q_i = Q$ where Q denotes the total mass (volume) of the system.
6. This ratio is used to convert concentration into content. The inverse ratio V/m is often termed "specific volume" and used to convert content into concentration.
7. m is the mass of the system, m_B and m_i are the masses of specified components. An analogous notation is used for amount of substance n and number of entities N .
8. m_s denotes the mass of the solvent.
9. Values of ratios are usually stated using a colon, such as 1.5 : 1 or 3 : 2 or 60 : 40.

1.8.3 Examples of Quantities Applied in Various Subdisciplines of Analytical Chemistry

Quantities specific to the different disciplines of *analytical chemistry* may be found in the various 'Colour Books' such as the IUPAC Green Book⁶ and the IUPAC-IFCC Silver Book,⁵ and in the respective chapters of this Compendium. The selection assembled in Table 1.8 provides the reader of analytical literature with a basic overview. *International System of Units* derived units with special names are listed in Table 1.10.

Table 1.8 Other quantities used in analytical chemistry.

Quantity or constant	Symbol	Definition (relating to specified component B, C)	SI unit	Note
time, duration	t		s	1
frequency (of periodic phenomenon)	ν, f	$\nu = 1/T$	$\text{s}^{-1} = \text{Hz}$	
period	T		s	2
angular frequency, angular velocity	ω	$\omega = 2\pi \nu$	s^{-1}	3
speed	v	$v = dl/dt$	m s^{-1}	
plane angle	$\alpha, \beta, \gamma, \dots$		rad, 1	4
solid angle	Ω	$\Omega = A/r^2$	sr, 1	5
force	F		$\text{N} = \text{m kg s}^{-2}$	
weight	G	$G = m g$	N	
standard acceleration of gravity $g_n = 9.80665 \text{ m s}^{-2}$ (defined) ⁶	g_n		m s^{-2}	
relative centrifugal force (rcf)	f_{rel}	$f_{\text{rel}} = m \omega^2 r/G$	1	6
moment of force, torque	M	$M = F \times l$	N m	
surface tension	γ	$\gamma = dW/dA$	N/m	5
pressure, stress	p	$p = F/A$	$\text{Pa} = \text{N m}^{-2}$	5, 7
viscosity (dynamic)	η		Pa s	
energy, work, heat	E, W, Q		$\text{J} = \text{N m}$	
electronvolt $\text{eV} = 1.602176634 \times 10^{-19} \text{ J}$ (constant usable as unit)	eV	$\text{eV} = (1 \text{ V}) e$	$\text{J} = \text{C V}$	8, 9

Table 1.8 (Continued)

Quantity or constant	Symbol	Definition (relating to specified component B, C)	SI unit	Note
power	P		$W = J s^{-1}$	
Planck constant $h = 6.62607015 \times 10^{-34} J s$	h		J s	8
molar gas constant $R \approx 8.314462618 J K^{-1} mol^{-1}$	R	$R = k N_A$	$J K^{-1} mol^{-1}$	8
Celsius temperature zero point at 273.15 K (defined) ⁶	θ, t		$^{\circ}C$	10
thermodynamic temperature	T		K	
standard temperature and pressure for gases (STP)		$\theta = 0^{\circ}C, P = 10^5 Pa$		
pH	pH, $p a_{H^+}$	$pH = -\log_{10} (a_{H^+})$	1	11
elementary charge $e = 1.602176634 \times 10^{-19} C$	e		C	8
Faraday constant $F \approx 96485.33212 C mol^{-1}$	F	$F = e N_A$	$C mol^{-1}$	8
electric charge	Q		$C = A s$	
electric current	I, i		A	
electric current density	J, j		$A m^{-2}$	
electric potential	V, Φ		$V = J C^{-1}$	
electric potential difference, tension	U		V	
electric field strength	E	$E = U/l$	$V m^{-1}$	
electric resistance	R	$R = U/I$	$\Omega = V A^{-1}$	
electric impedance	Z	$Z = R + iX$	Ω	12
electric resistivity	ρ		Ωm	
electric conductance	G		$S = \Omega^{-1}$	
electric conductivity	σ		$S m^{-1}$	
electric capacitance	C		$F = C V^{-1}$	
magnetic field strength	H		$A m^{-1}$	
magnetic flux density, magnetic induction	B		$T = V s m^{-2}$	13
activity of a radioactive material, activity	A	$A = -dN_B/dt$	$Bq = s^{-1}$	14, 15
decay (rate) constant	λ	$\lambda = A/N_B$	s^{-1}	14
specific activity	a	$a = A/m$	$Bq kg^{-1}$	16
isotopic ratio	R	$R = N_B/N_C$	1	
abundance of isotope iE in element E:				17
isotope mole fraction.	$x({}^iE)$	$x({}^iE) = n({}^iE)/n(E)$	1	
isotope number fraction	$X({}^iE)$	$X({}^iE) = N({}^iE)/N(E)$	1	
half-life	$t_{1/2}, T_{1/2}$		s	18
absorbed dose	D		$Gy = J kg^{-1}$	
dose equivalent	H		$Sv = J kg^{-1}$	
speed of light	c		$m s^{-1}$	
speed of light in vacuum $c_0 = 2.99792458 \times 10^8 m s^{-1}$	c, c_0		$m s^{-1}$	8
wavelength	λ		m	
wavenumber	$\tilde{\nu}, \sigma$	$\tilde{\nu} = \lambda^{-1}$	m^{-1}	19
frequency (of electromagnetic radiation)	ν	$\nu = c \lambda^{-1}$	Hz	
refractive index	n	$n = c_0/c$	1	20
radiant energy	Q, W		J	21
radiant power, (radiant energy per time)	P	P	$W = J s^{-1}$	22
radiant intensity	I_e	$I_e = dP/d\Omega$	$W sr^{-1}$	23
irradiance, intensity	I	$I = dP/dA$	$W m^{-2}$	21, 23
luminous intensity	I_v		cd	20
luminous flux	Φ_v		$lm = cd sr$	21
illuminance	E_v	$E_v = d\Phi_v/dA$	$lx = lm m^{-2}$	5, 21
resolution	$\delta\tilde{\nu}$		m^{-1}	24
transmittance	T	$T = P_{transmitted}/P_0$	1	

Table 1.8 (Continued)

Quantity or constant	Symbol	Definition (relating to specified component B, C)	SI unit	Note
reflectance	R	$R = P_{\text{reflected}}/P_0$	1	
absorptance	α	$\alpha = 1 - T$	1	
absorbance	A	$A = \varepsilon c l$	1	
decadic absorbance	A_{10}	$A_{10} = -\log_{10} T$	1	
Naperian absorbance	A_e	$A_e = -\ln T$	1	
absorption coefficient	ε	$\varepsilon = A/cl$		25
absorption index	k	$k = A_e/(4\pi l\tilde{\nu})$	1	
complex refractive index	\hat{n}	$\hat{n} = n + ik$	1	
angle of optical rotation	α		1, rad	3
specific optical rotatory power	$[\alpha]_D^\theta$	$[\alpha]_D^\theta = \alpha/\rho l$	rad m ² kg ⁻¹	4, 26
catalytic activity	z_E		kat = mol s ⁻¹	
mass flux	q_m	$q_m = dm/dt$	kg s ⁻¹	

1. Non-SI units of time accepted for use with the SI are minute (min = 60 s), hour (h = 3600 s), and day (d = 86 400 s); while week, month, year are not accepted for use with SI units.

2. Time between identical events in periodic phenomena.

3. The unit Hz is not to be used for angular frequency.

4. The plane angle is often given in degree (°) where 1° = (π/180) rad; the degree can be divided decimally or in minute (1' = (1/60)°) and second (1'' = (1/60)')

5. A denotes (surface) area.

6. The *ref* ratio is used to characterize the effect of centrifuging a sample (frequency ν , radius r) in comparison to the gravitational acceleration g :

$$f_{\text{rel}} := \omega^2 r/g = 4\pi^2 \nu^2 r/g \approx (4 \text{ s}^2/\text{m})\nu^2 r.$$

In practice, the rotational frequency ν of the centrifuge is often given in “revolutions per minute” (rpm) and r is in the order of millimeters, then *ref* can be re-written as $f_{\text{rel}} \approx 1.12 \{r\}_{\text{mm}} (\{\nu\}_{\text{rpm}}/1000)^2$, where the braces indicate the numerical value of the quantity when measured in the unit stated as subscript.

7. Pressure is often expressed in the non-SI unit bar, where

$$1 \text{ bar} = 10^5 \text{ Pa and } 1 \text{ mbar} = 10^{-3} \text{ bar} = 100 \text{ Pa} = 1 \text{ hPa};$$

$$\text{further } 1 \text{ atm} = 1.01325 \text{ bar and } 1 \text{ atm} = 760 \text{ Torr.}$$

$$1 \text{ Torr} \approx 1 \text{ mmHg and } 1 \text{ psi} \approx 68.95 \text{ mbar.}$$

8. The fixed constants defining the SI are given in Table 1.9 of Section 1.8.5. They do not carry any measurement uncertainty.

9. The electronvolt, symbol “eV”, is a non-SI unit accepted for use with the SI and may be combined with the SI prefixes given in Table 1.3.

10. Degree Celsius is an SI-derived unit with special name and term (see Table 1.10).

11. a_{H^+} is the activity of the hydrogen ion in solution.

12. The reactance $\text{Im}(Z) = X = (U/I) \sin \delta$ where δ is the loss angle.

13. This quantity should not be termed “magnetic field”.

14. N_B denotes the number of decaying entities.

15. Activity referred to a radio nuclide is sometimes incorrectly termed radioactivity.

16. The term “massic activity” is also used.

17. Since all isotopes of the given element are known $n(\text{E}) \equiv \sum n(\text{E})$ and $N(\text{E}) \equiv \sum N(\text{E})$

18. Half-lives of long-lived isotopes are commonly given in the non-SI unit years.

19. In infrared and Raman spectroscopy wavenumbers $\tilde{\nu}$ are typically given in cm⁻¹.

20. The speed of light within the medium is denoted by c .

21. The symbols for the quantities such as radiant energy are also used for the corresponding quantities concerning visible radiation, *i.e.* luminous quantities and photon quantities. Subscripts e for energetic, v for visible and p for photon may be added. The units used for luminous quantities are derived from the base unit candela (cd).

22. Radiant intensity is the radiant power per solid angle in the direction of the point from which the source is being observed.

23. The intensity or irradiance I is the radiation power per area that is received at a surface. This quantity must be distinguished from radiant intensity I_e which characterizes the source.

24. The correct definition of resolution depends on the line shape, but usually resolution is taken as the full line width at half maximum intensity (FWHM).

25. The unit depends on whether mass concentration or amount-of-substance concentration is used, the numerical value depends also on the base of the logarithm.

26. θ denotes Celsius temperature, ρ mass density.

1.8.4 Adjectives Modifying Quantity Terms

A *quantity* that is additive for independent, non-interacting subsystems is termed “extensive”; examples are mass and volume. A quantity that is independent of the extent of the *system* is termed “intensive”, such as mass concentration, temperature, and pressure.

The adjective “specific” before the term of an extensive quantity is used to mean “divided by mass of system”.

Other admitted modifiers to denote quantities derived by division with mass, volume, area, length, and number of entities are massic, volumic, areic, lineic, and entitic, respectively. In most cases such terms are used in specialized context, and a broader community may not be familiar with the meaning.

The adjective “molar” referring to division by amount of substance is often found, even though it violates the principle that the term of a quantity should not be mixed with the term of a unit. See ref. 6.

1.8.5 Defining Constants of the International System of Units

On 20 May 2019 the revision of the *International System of Units (SI)* came into force.³² The SI is now defined in terms of a set of seven defining constants which are fixed so do not carry any *measurement uncertainty*. The complete *system of units* can be derived from the fixed values of these defining constants, expressed in the *units* of the SI. See Table 1.9.

Table 1.9 The defining constants of the SI.

Defining constant	Symbol	Numerical value	Unit
the unperturbed ground state hyperfine transition frequency of the caesium 133 atom	$\Delta\nu_{\text{Cs}}$	9192631770	Hz
the speed of light in vacuum	c	299792458	m s^{-1}
the Planck constant	h	$6.62607015 \times 10^{-34}$	J s
the elementary charge	e	$1.602176634 \times 10^{-19}$	C
the Boltzmann constant	k	1.380649×10^{-23}	J K^{-1}
the Avogadro constant	N_{A}	$6.02214076 \times 10^{23}$	mol^{-1}
the luminous efficacy of a defined visible radiation	K_{cd}	683	lm W^{-1}

1.8.6 SI-Derived Units with Special Terms and Symbols

See Table 1.10

Table 1.10 SI-derived units with special names and symbols.

Name of unit	Symbol	Expressed in terms of other SI units	Related quantity	Symbol
becquerel	Bq	s^{-1}	activity of a radionuclide	A
coulomb	C	A s	<i>electric charge</i>	Q
degree Celsius	$^{\circ}\text{C}$	K	Celsius temperature	t
farad	F	C V^{-1}	capacitance	C
henry	H	Wb A^{-1}	inductance	L
hertz	Hz	s^{-1}	frequency of a periodic phenomenon	f, ν
gray	Gy	J kg^{-1}	absorbed dose	D
joule	J	N m	energy, work, amount of heat	E, W, Q
katal	kat	mol s^{-1}	catalytic activity	z_{E}
lumen	lm	cd sr	luminous flux	Φ_{v}
lux	lx	lm m^{-2}	illuminance	E_{v}
newton	N	m kg s^{-2}	force	F
ohm	Ω	V A^{-1}	electric resistance	R
pascal	Pa	N m^{-2}	pressure, stress	p
radian	rad	1	plane angle	$\alpha, \beta, \gamma, \dots$
steradian	sr	1	solid angle	Ω
siemens	S	Ω^{-1}	electric conductance	G
sievert	Sv	J kg^{-1}	dose equivalent	H
tesla	T	Wb m^{-2}	magnetic flux density, magnetic induction	B
volt	V	W A^{-1}	electric potential difference	U
watt	W	J s^{-1}	power, radiant flux	P
weber	Wb	V s	magnetic flux	Φ

1.9 Checklist for Making Measurements in Analytical Chemistry

This checklist will lead to a *measurement result* that has *metrological traceability* and appropriate *measurement uncertainty*.⁵⁹

- Definition of *measurand*, intended use of measurement results, and *target measurement uncertainty*. This will include a statement of the individual *quantity* to be measured, including *system*, relevant *components*, and *kind of quantity*, with a statement of the *measurement model* or *measurement function* and a description of the *measuring system* as well as of the *measurement procedure*, including whether any *correction* is to be made for *recovered quantity value ratio*. The target measurement uncertainty will influence the stringency of the *metrological traceability chain*; the end-user's measurement uncertainty will be larger than that associated with the *calibrator(s)* used to establish metrological traceability.
- Selection of metrological reference in the form of a *measurement unit*, measurement procedure, or *measurement standard* (see Note 3 to *calibration hierarchy*). Establishment of metrological traceability can only be achieved to an existing and documented metrological reference.
- Selection of *calibration hierarchy*. By making the selection of the end-user's working calibrator on available documentary evidence, the calibration hierarchy is fixed. Attention should also be paid to the *calibration* and metrological traceability of measurement results for *input quantities in a measurement model* and *influence quantities*, including those measured by accessory equipment such as balances, thermometers, and volumetric ware.
- Selection of suitably validated measurement procedure. The analytical chemist should check whether a previously validated measurement procedure can be implemented in the analyst's laboratory and in the positive case verify its performance.
- Acquisition and verification of end-user's calibrator. Such a calibrator should be verified for absence of changes during transport and storage, validated for *commutability of a reference material*, have documented metrological traceability of its stated *quantity value* and associated measurement uncertainty.
- End-user's *measurement* on system or *sample* to obtain measurement result, including measurement uncertainty, based on an *uncertainty budget*.
- Documentation and report of metrological traceability. This requires readily available evidence, *e.g.*, certificates or statements of metrological traceability for all calibrators used, and *calibration certificates* for equipment.

The purpose of performing a measurement is to provide information, in the form of a measurement result, on the value of a measurand embodied in a specified system. The amount of information given directly varies with the intended use of the measurement result. When only the *measured quantity value* is presented, the associated measurement uncertainty and metrological traceability should be available. The documentation can take the form of a 'certificate of analysis', 'test report', 'measurement report' 'calibration certificate' or more extensively a 'certification report'.^{3,68} A certification report specifies all details necessary to understand the production, properties, and use of the calibrator (measurement standard or *certified reference material*), its value, measurement uncertainty, and metrological traceability.

The documentation of metrological traceability of the measurement result is essential because it

- underpins the authority of the measurement result by demonstrating how the result has been arrived at through the use of calibrators and measurement procedures;
- identifies the metrological reference needed to achieve metrological comparability of measurement results for quantities of the same kind; and
- shows the elements in the uncertainty budget of the measured quantity value that are necessary for the calculation of the final measurement uncertainty.

1.10 Presentation of Quantities and Their Values

Most of what appears in this section can be found in the IUPAC Green Book.⁶ The reason to insist that properties, units, symbols, and terms should be fashioned and presented according to generally accepted conventions is that science depends on reliable communication, and only by using the generally agreed form the message will be unmistakable.

1.10.1 Quantity and Value

Analytical chemistry is mostly about measuring the value of a *unitary quantity*. A *quantity* that is intended for *measurement* is termed a *measurand* and this is specified by the *kind of quantity* and the *embodying system* including any relevant *component*. An example would be mass concentration of sodium chloride dissolved in water. A *measured quantity value* of a unitary measurand in principle consists of two parts: *numerical quantity value* and *measurement unit*. Examples: 3.4 mg, 0.12 mL, 0.98 g g⁻¹, 100 mV s⁻¹, 7.2 %, 5.0 × 10⁻¹¹ mol L⁻¹.

1.10.2 Numerical Quantity Value

This should be given with a number of significant digits (decimal places) appropriate with regard to the *measurement uncertainty*. In order to avoid insignificant figures, a suitable multiple or submultiple of the *unit* as indicated by a prefix to the unit symbol (see *International System of Units* Note 5) or scientific notation (using a power of 10 as factor) should be applied. Examples: 0.23 μA = 230 nA = 2.3 × 10⁻⁷ A, but not 0.0000023 A.

It must be noted that the numerical value of a quantity value depends on the unit chosen, in the above examples 0.23, 230 and 2.3 × 10⁻⁷, respectively, and that the power-of-10 factor is considered a part of the numerical value.

1.10.3 Measurement Unit

When possible, SI units or 'non-SI units accepted for use with the SI'³² should be used. The litre is such an accepted non-SI unit symbolized by l or L, where L is recommended to avoid confusion with the number 1 (one). The SI unit of time is the second (symbol s, not sec, sec., secs), while the units minute (min), hour (h), and day (d) are non-SI units accepted for use with the SI.³²

The unit in a *measured value* of a *unitary quantity* by itself does not indicate the *quantity* concerned. For example, mass concentration and mass density both have the unit kg m⁻³. All the more it is important to state the quantity when a measured value is presented, and in case of a fraction to clarify its type such as mass fraction.

Note that "one", symbol "1", can be considered a *base unit* in the SI, but usually the symbol of this unit is omitted. There are many quantities using the unit 1, for example: mass fraction kg kg⁻¹, amount-of-substance fraction mol mol⁻¹.

The units per cent, %, or per mille (or per mil), ‰, are accepted by ISO, whereas the units ppm and ppb that are used widely in *analytical chemistry* are deprecated by IUPAC⁶ and ISO.

Composite units (such as g L⁻¹) should not be separated by other information, *e.g.*, g of salt L⁻¹.

Both the term and the symbol of a unit are always written in upright (roman) type, not in bold or italics. As a rule, terms for units start with a lower-case letter. Units termed after persons follow this rule, but when symbolized, the first letter is capitalized. Examples: dalton, Da; ampere, A; volt, V; becquerel, Bq. The litre, l or L is an exception, where the capital L is used when lower case l might be confused with the number 1.

Ordinal quantities and *nominal properties* have no units.

1.10.4 Spacing

In the expression of a *quantity value* of a *unitary quantity* there is a space between the number and the unit symbol, and between different unit symbols, but not between a prefix and unit. Examples: 12 g, 99 %, 25 °C, 14 mm, 1.3 $\mu\text{mol L}^{-1}$.

As an alternative to using negative powers of units, a solidus (/) can be employed. Examples: $1 \text{ N} = 1 \text{ m kg s}^{-2} = 1 \text{ m kg/s}^2$, $1 \text{ g g}^{-1} = 1 \text{ g/g} = 1$.

1.10.5 Measurement Result

The *measured quantity value* should be accompanied by information on the *measurement uncertainty* to specify the interval of possible values. The contribution to the uncertainty from all relevant sources should be presented in an *uncertainty budget*. The evaluation of measurement uncertainty is described in the GUM³⁴ and the Eurachem/CITAC Guide CG4.⁴⁷

1.10.6 Measurement Uncertainty

The estimated value of the uncertainty is given either as a *standard uncertainty*, u (a measurement uncertainty expressed as a standard deviation), or as an *expanded measurement uncertainty* U (with a coverage factor $k > 1$). The standard deviation (s) of values obtained by repeated *measurements* should not be termed measurement uncertainty but standard deviation. In all reports, papers, and theses it should be made clear for which *coverage probability* the uncertainty is being reported.

Measurement uncertainty is usually stated with no more than 2 significant digits, the decimal places of the *numerical quantity value* should be given correspondingly. Examples of presentation of a *measurement result*:

(8.89 \pm 0.24) g with expanded uncertainty ($k = 2$) for a coverage probability of approximately 95 %; 8.89 g ($u = 0.12$ g); 8.89 g ($s = 0.10$ g, $n = 4$);

in case the uncertainty is much smaller than the *quantity value*, the following notation is useful: 100.02147(35) g, where the number in parentheses denotes the standard uncertainty, which is applied to the last significant digits, *i.e.*, 100.02147 g \pm 35 mg.

1.10.7 Symbol for Quantity

To avoid writing the full term of a *quantity*, a symbol may be given instead. Recommended symbols for most quantities are given in the ISO 80000 series³¹ and the Green Book⁶ and should be preferred. Some are given in Section 1.8. If there are reasons to choose other symbols, their meaning must be explained. Symbols that apply to specified entities should always be indicated whether by a subscript or in parentheses, *e.g.*, amount of substance of entity B, n_{B} or $n(\text{B})$. When the chemical composition is written out, parentheses should be used, $n(\text{O}_2)$.

1.10.8 Italic and Roman Font Style

Symbols for *quantities*, defining and reference constants^{35,69} and variables are in italics, except for “pH”. Superscripts and subscripts are in roman font unless they are quantity symbols themselves or variables representing a numerical index. Examples: N_{A} Avogadro constant; m_i mass of the i^{th} sample; λ_{max} *wavelength* at maximum *absorbance*.

1.10.9 Tables and Diagrams

Quantity values in a table or a diagram are usually given by their *numerical values* in the columns or at the axes, respectively, while in the column heads and the axes labels the symbol for the *quantity* and its *unit* are shown divided by a solidus (/). For *derived units* parentheses are necessary. Examples: m/kg ; $c/(\text{mmol L}^{-1})$.

Table 1.11 Calibration data for the electrochemical measurement of mass concentration γ of cadmium in solution; j is the electric current density.

$\gamma/(\text{ng L}^{-1})$	$j/(\mu\text{A cm}^{-2})$
0.6	0.2
1.5	0.8
2.4	1.3
...	...
11	4.3
14	4.7
21	5.1
34	6.1
49	6.3

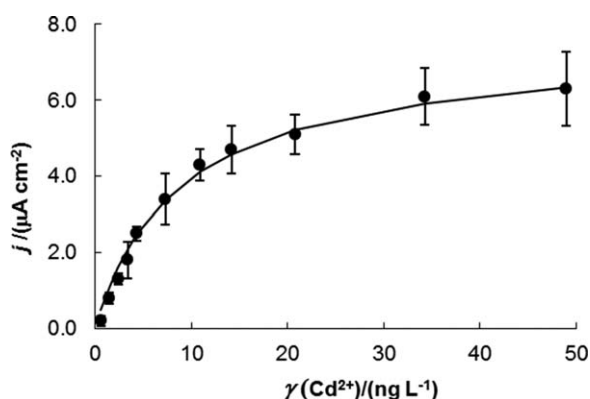


Figure 1.1 Calibration curve for the electrochemical measurement of the mass concentration γ of cadmium in solution; error bars indicate the $\approx 95\%$ coverage interval being \pm two times the standard uncertainty.

See Table 1.11 and Figure 1.1 for an example of a *calibration* of the electrochemical *measurement* of the mass concentration of cadmium in solution. Tables and figures should be accompanied by explicative captions.

For straight lines, a function $y = ax + b$ is often given either in the caption or as an insert in the diagram, where for the sake of simple notation y and x refer to numerical values at the respective axes.

1.10.10 Equations

Equations such as a *measurement function*, should deal with *quantity values*, *i.e.*, the product of numbers and *quantity units*, rather than with *numerical values* and unit-conversion factors. Applying the ordinary rules of algebra to quantity values is known as *quantity calculus* and has particular advantages in facilitating the problems of converting between different units and different *systems of units*. In practice, it is helpful that such an equation is independent of the choice of units and offer the essential check of whether the *quantity dimensions* are the same on either side of the equal sign. Equations based on numerical values (omitting units) are convenient in routine work, but not appropriate for a wider audience, for example in scientific literature.

Terms of quantities (words) or multi-letter abbreviations of terms should not be used in place of symbols, for example in equations.

Regarding a mathematical expression, there should be spaces on both sides of most signs for dyadic operators such as $+$, $-$, \pm and \times (but not for the solidus), and for relations, such

as =, <, ≤, but not after monadic operators such as + and – (e.g., +25 °C). The centre (multiplication) dot is usually also written without spaces (e.g., m·kg·s⁻³·A⁻¹).

When × is used in a number before a power of ten, e.g., 5.3×10⁻⁵, there are no spaces.

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