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Abstract. The quantities used for expressing the composition of mixtures are described and classified into five groups: ratios, fractions, concentrations, molality and contents. The international recommendations are compared with current practice where discrepancies are common.

1. Introduction

In many fields of science and even more so in applied fields we deal with mixtures and are interested in their qualitative and quantitative composition. Since the fields of application span an extremely wide range including solid-state physics, astronomy, environmental sciences, medicine, agriculture, ..., different terminologies and symbolisms have developed. The present article describes a classification of the physical quantities used to express the composition of mixtures on the basis of international recommendations [1-3] and standards [4, 5] designed to bring order and better understanding to the problem and to draw attention to the various inconsistencies we encounter in practice but should try to avoid.

2. Recommendations

When a sample consists of two or more pure substances we say that it is a mixture. A solution is a special case, in which one substance is treated differently from the others. Thus in general a mixture consists of two or more substances, and a solution consists of a substance called the solvent (usually, but not necessarily, the major constituent of the mixture and usually, but not necessarily, a pure substance) and one or more substances called the solutes [6]. The individual substances in a mixture are often called the components of the mixture in the sense of being its composite parts, but in thermodynamics the term "component" has the very specific meaning of a chemically independent constituent substance in the system [7]. As this might lead to confusion when analysing complex reacting mixtures where substances dissociate into different reacting species [8], we avoid the term component in this discussion and focus only on the different quantities used to express the composition, not on the processes and the interdependences in reacting systems. The quantities are, of course, applicable to any chemical species in the system and some of them even to entities such as $\frac{1}{2}\,Ca^{2+}$, $\frac{1}{3}\,PO_4^{3-}$, or nitrogen atoms irrespective of the species of which they are part.

The size of a sample, i.e. how large it is, can be described by any of the four extensive quantities: mass (symbol: m), volume (symbol: V), number of molecules or other entities building up the sample (symbol: N), or chemical amount (amount of substance, previously often called the number of moles, symbol: n). Which of these is chosen in a specific case is a matter of convenience. Mass and volume have the advantage of being easier to measure, but the number and chemical amount of entities are more convenient in theoretical considerations, for mutual comparisons and understanding of chemical equilibria, and for rates of reactions. It is important to note here that while mass, number and amount of entities are conserved quantities in that the sum of the quantities for all the individual composite parts of the system is equal to the quantity for the system as a whole $\sum_j x_j = x_{\mathrm{tot}}$ ($x = m$, N or n), volume is not. For fluids (liquids and gases) the sum of volumes of the individual composite parts is not generally equal to the total volume of the mixture. In addition, volume depends on temperature and pressure, and special care has to be taken to avoid misunderstandings and errors when using quantities defined in terms of volume.

The composition of a mixture is expressed by an intensive quantity since the composition does not depend on the size or extent of the sample. Such intensive quantities can be obtained by division of any of the above extensive quantities by another extensive quantity for the whole sample or for another

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substance in the mixture. Again there are several ways in which one can do this depending on convenience either of measurement or of application. The quantities obtained in this way can be divided into four groups: *ratios, fractions, concentrations* and *molality*. In clinical chemistry, a fifth group of quantities is used: these are called *contents* [3].

2.1 Ratios

For a mixture of two or more substances, it is sometimes convenient to refer to the ratio of two substances. We denote the substances with indices i or j but when it is necessary to specify the molecules (entities in general), i.e. whenever amounts or numbers of molecules are used, we use the index B for the general substance and A for the solvent. For example, while it is sufficient to say that the mass of sulphur in a sample is 256 mg, $m_{\rm S} = 256$ mg, when we talk about numbers and amounts of entities we have to specify the entities counted. Thus if the amount of sulphur with respect to S_8 molecules (for short the amount of S_8 molecules) is 1 mmol, the amount of atoms is $n_{\rm S} = 8$ mmol. The meaning of the subscript S is not the same in the two cases. When it refers to mass it denotes the substance sulphur: when it refers to amount it specifies the entity counted. Depending on which extensive physical quantity is used to express how much of a substance we have, we can distinguish three types of ratio:

Name	Symbol	Definition
Mass ratio	$\zeta_{i,j}$	$\zeta_{i,j} = m_i/m_j$
Volume ratio	$\psi_{i,j}$	$\psi_{i,j} = V_i/V_j$
(Chemical) amount ratio, mole ratio, number ratio	$r_{\rm B,A}$	$r_{\rm B,A} = n_{\rm B}/n_{\rm A} = N_{\rm B}/N_{\rm A}$

Ratios are not commonly used. Neither the IUPAC nor the IUPAP explicitly recommends symbols for these quantities. The ISO [4.i] recommends only the amount ratio (calling it the mole ratio). The other symbols listed were adopted from the German standard [5] which, in addition, recommends R for number ratio although it is identical with the amount ratio r. It is important to note here that when ratios are used it has to be made clear which substance of the mixture is chosen as reference. In solutions this is usually the solvent. In this case the second index is often left out, but in general it has to be specified. Sometimes in the description of a preparation procedure it is said that two liquids are taken in a particular volume ratio, for instance, 1 : 5. Mass and amount ratios are often used to describe the quantitative relationship between different substances in reaction mixtures, but the symbols are hardly ever used.

2.2 Fractions

A fraction describes how much of the total property of a sample is contributed by one of its constituent substances. Just as for ratios, we can distinguish three types of fraction:

Name	Symbol	Definition
Mass fraction	w	$w_i = m_i/\sum m_j$
Volume fraction	φ	$\varphi_i = V_i/\sum V_j$
(Chemical) amount fraction, mole fraction, number fraction	x	$x_{\rm B} = n_{\rm B}/\sum n_j = N_{\rm B}/\sum N_j$

The denominator in all these definitions refers to the sum over all the composite parts including the one in the numerator. Since the number of entities is proportional to the chemical amount of entities and the proportionality constant is equal for all substances, the amount fraction is identical with the number fraction. The German standard [5], however, lists the number fraction separately with the symbol X. Fractions are used very frequently to express how much of a substance is contained in a sample. They are all dimensionless quantities with values between 0 and 1 and are most commonly expressed in forms of the percent, % ($= 10^{-2}$) and, for lower values, part per million, ppm ($= 10^{-6}$). It should be noted that the quantities in the denominator refer to values prior to mixing. This is important when describing volume fraction, since the sum of volumes of all composite substances does not generally equal the total volume of the mixture, so a confusion with volume concentration, as described below, is possible.

2.3 Concentrations

Concentrations are physical quantities describing the ratio of one of the extensive quantities of a single substance (mass, volume, chemical amount or number of entities) to the total volume of the mixture, V. Thus there are four kinds of concentration:

Name	Symbol	Definition	SI unit	Common units
Mass concentration	γ, ρ	$\gamma_i = m_i/V$	kg m^{-3}	g/L = g dm^{-3}
Volume concentration	σ	$\sigma_i = V_i/V$	1	1
Amount concentration	c	$c_{\rm B} = n_{\rm B}/V$	mol m^{-3}	mol/L = mol dm^{-3}
Number concentration	C	$C_{\rm B} = N_{\rm B}/V$	m^{-3}	cm^{-3}

All these concentrations have different dimensions and different units. Mass concentration is a practical quantity, especially for preparing solutions, because both the mass of the solute and the volume of the solution can be measured easily. The commonly used units are g/L, g/100 mL, etc. Volume concentration is easily confused with volume fraction and indeed, when the sum of volumes of the composite substances is equal to the total volume of the mixture, the two quantities become equal. When using volume concentrations this has to be made clear: for this reason their use is best avoided. The chemical amount concentration (amount of substance concentration, previously called molarity) is the most frequently used quantity for expressing the composition of solutions in chemistry since it enables a quick and chemically meaningful comparison of different solutions, and rates and equilibria are directly related to amount concentration. When there is no risk of ambiguity the amount concentration may be abbreviated to the single word "concentration". The term previously used for amount concentration, molarity, and the corresponding symbol M for mol/L are no longer recommended, although in fact they are still widely used. The most common units for amount concentration are mol/L (= mol dm^{-3}), and its decimal sub-multiples mmol/L, µmol/L, etc. Number concentration is usually used in describing gaseous mixtures and the common unit is then cm^{-3}.

2.4 Molality

The molality is defined as the amount of solute entities divided by the mass of the solvent. Its recommended symbol is m. The alternative symbol, b, is used, as here, when there is a possibility of confusion with mass:

$$b_{\mathrm{B}} = n_{\mathrm{B}}/m_{\mathrm{solv}}.$$

Indeed the German standard [5] recommends only b as symbol for molality and the new International Standard ISO 31-8 [4.i] lists b before m. Molality is often used in thermodynamic treatments and has the advantage over amount concentration that it is temperature independent. The most common unit is mol/kg.

2.5 Contents

Contents are quantities describing the ratio of one of the extensive quantities of a substance in a mixture (mass, volume, chemical amount or number of entities) to the total mass of the mixture, m. Since the sum of masses of all substances in a mixture is equal to the total mass of the mixture, mass content is identical with mass fraction and is therefore redundant. Thus there remain only three contents:

Name	Symbol	Definition	SI unit
Volume content	κ	$\kappa_i = V_i/m$	m^3 kg^{-1}
Amount content	k	$k_{\mathrm{B}} = n_{\mathrm{B}}/m$	mol kg^{-1}
Number content	K	$K_{\mathrm{B}} = N_{\mathrm{B}}/m$	kg^{-1}

Contents are rarely used in chemistry, and not listed in the major documents on quantities and units [1, 2, 4]. Two such contents (number content and amount of substance content) are mentioned in the document on clinical chemistry [3], but no symbols are recommended. The symbols listed here were chosen arbitrarily so that the defining equations could be put in written form.

2.6 Example

By mixing 70 mL of ethanol and 30 mL of water at 20 °C one obtains 96,8 mL of solution. The densities of ethanol and water at 20 °C are 0,7893 g cm^{-3} and 0,9982 g cm^{-3}, respectively, so that all the quantities describing the composition of this mixture can be calculated:

Ratios	
Volume ratio	ψ(EtOH, H_2O) = 7 : 3
Mass ratio	ζ(EtOH, H_2O) = 1,84 : 1 ≈ 11 : 6
Amount ratio	r(EtOH, H_2O) = 0,721 : 1 ≈ 3 : 4
Fractions	
Volume fraction	φ(EtOH) = 70 %
Mass fraction	w(EtOH) = 64,8 %
Amount fraction	x(EtOH) = 41,9 %
Concentrations	
Mass concentration	γ(EtOH) = 571 g/L
Volume concentration	σ(EtOH) = 0,723
Amount concentration	c(EtOH) = 12,4 mol/L
Number concentration	C(EtOH) = 7,47 × 10^{21} cm^{-3}
Molality	
Molality	b(EtOH) = 40 mol kg^{-1}
Contents	
Volume content	κ(EtOH) = 822 mL kg^{-1}
Amount content	k(EtOH) = 14,1 mol kg^{-1}
Number content	K(EtOH) = 8,49 × 10^{21} g^{-1}

3. Common practice

Having defined and grouped all the quantities, it is easy to spot those which deviate from recommended usage. Here, we comment on some of the most frequent deviations.

The term "concentration" is often used as a general term for any of the quantities listed here. Thus fractions are often called concentrations and one can deduce that the intended meaning is a fraction only from the units used. Furthermore, since all fractions are of dimension one (dimensionless), and hence are expressed in the same units, a decoration is frequently added to the symbol of the unit in order to specify which fraction is meant. This practice is highly deprecated since symbols of units should never be changed and never used to describe the quantity being measured. Instead of writing "the concentration is 1 ppmv", we should write "the volume fraction is 1 ppm"; instead of "concentration of 12 %w/w" we should write "mass fraction of 12 %", etc. In dilute aqueous solutions, mass concentrations expressed in milligrams per litre are almost equal to mass fractions expressed in parts per million. Here again expressions are found such as "concentration of nickel equals 2,6 ppm" instead of "mass concentration of nickel equals 2,6 mg dm^{-3}".

In atmospheric chemistry the term "mixing ratio" is often used to denote a volume fraction or number fraction. It is obvious that even if the term were applied to a ratio, say with respect to standard dry air (which is never mentioned, but is nearest to what is meant), the attribute specified by the word "mixing" brings no additional information and the ambiguity, as to whether a mass, volume or number ratio is meant, remains [9]. Once again, authors resolve the problem by the prohibited decoration of unit symbols.

Another common problem is the use of units for the description of fractions in terms of sub-multiples of one in circumstances where the sub-multiples are treated as units in a system of counting. The most frequently used unit of this kind is the percent with symbol % standing for 0,01 or 10^{-2}. It is the only such unit accepted by the ISO [4], but is not even recognized by the Comité Consultatif des Unités. The IUPAC [1] also recommends use of the unit part per million, ppm ($=10^{-6}$), which is also used in CODATA documents [10] and as "part in 10^6" in the IUPAP document [2] for expressing the relative uncertainties of precise measurements. In practice, however, one encounters a much larger variety of units and symbols of this kind, and this necessarily leads to confusion. In continental Europe the permille, ‰ ($=10^{-3}$) is a common unit for expressing the mass fraction of alcohol in blood or the salinity of sea water, while in other parts of the world parts per thousand, abbreviated to ppt, are used. For very small quantities, a common form based on the American system of counting is to use parts per billion, ppb ($=10^{-9}$), parts per trillion, ppt ($=10^{-12}$). … These are often used without realizing that in Europe a system of counting was established long ago in which a billion stands for $(10^6)^2=10^{12}$, a trillion for $(10^6)^3=10^{18}$. … This usage is slowly fading in the United Kingdom, but it is bound to stay in continental Europe, where most languages have their own names for numbers of the type $10^3\times(10^6)^n$ which, translated into English, might read milliard, billiard, trilliard. … No international recommendation for such expressions is likely to be agreed so a different system based on SI prefixes would be most welcome. The present status and some possible solutions for consideration as future recommendations are summarized in Table 1.

Table 1.

Value	Symbol (present)		Symbol (to consider for future)		
	Practice	Recommended	Version 1	Version 2	Version 3
10^{-2}	%	%	%	%	%
10^{-3}	‰, ppt		‰	‰	mI
10^{-6}	ppm	(ppm)	ppM	ppm	µI
10^{-9}	ppb		ppG	ppg	nI
10^{-12}	ppt		ppT	ppt	pI
10^{-15}	ppq		ppP	ppp	fI

The ideal situation where practice and recommendation are in agreement can be found only with the use of percent. The parentheses around the symbol ppm denote that the ISO does not recommend its use. The three proposed versions for the future are based on SI prefixes. Version 1 is based on prefixes for multiples (mega, giga, tera and peta) with an unusual use of the prefix which stands on its own (e.g. part per mega) at the end of the expression. Version 2 uses the same system with lower-case letters, but with the advantage that it conforms to current practice in two instances. Version 3 makes proper use of the symbols for prefixes, but introduces a new symbol I (or Roman one) for one. The central purpose of this paper is to recommend that international commissions issuing recommendations should consider this and other proposals, consult with practising scientists and propose a solution acceptable to the majority.

4. Conclusion

The term "concentration" has two recommended meanings: (i) the name for a group of four quantities referring to the total volume of a mixture; and (ii) the short form for amount (of substance) concentration. Its use with a third, more general, meaning for any quantity describing the composition of a mixture is highly deprecated since it leads to confusion and a prohibited deformation of the symbols used for units. Adherence to common recommendations by international organizations and scientific unions on the use of quantities and units could bring coherence and avoid misunderstandings in communication between scientists from different backgrounds. An effort should therefore be made by all scientists, especially those involved in interdisciplinary research, to become familiar with the recommendations concerning units and to follow them whenever possible. International commissions on the other hand should seek solutions to confusing issues, consult as many scientists as possible and try to produce recommendations which are acceptable to those involved.

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   (d) ISO 31-3: 1992 Quantities and Units – Mechanics
   (e) ISO 31-4: 1992 Quantities and Units – Heat
   (f) ISO 31-5: 1992 Quantities and Units – Electricity and Magnetism
   (g) ISO 31-6: 1992 Quantities and Units – Light and Related Electromagnetic Radiations
   (h) ISO 31-7: 1992 Quantities and Units – Acoustics
   (i) ISO 31-8: 1992 Quantities and Units – Physical Chemistry and Molecular Physics
   (j) ISO 31-9: 1992 Quantities and Units – Atomic and Nuclear Physics
   (k) ISO 31-10: 1992 Quantities and Units – Nuclear Reactions and Ionizing Radiations
   (m) ISO 31-11: 1992 Quantities and Units – Mathematical Signs and Symbols for Use in Physical Sciences and Technology
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