





LETTER

Expressing the Unit of Measurement in Analytical Chemistry

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Units in Analytical Chemistry

Analytical chemistry is a measurement science that provides both qualitative and quantitative data across various areas, including basic science, industry, medicine, and space exploration. The subject of analytical procedures in multiple fields of analytical instrumentation enables the determination of the composition of mixtures containing two or more components.¹ So, we not only detect the composition but also specify the amount of the compound of interest. An example is the analysis of a milk sample to quantify the calcium concentration. In this context, milk is the sample analyzed, while calcium is the analyte being determined.² In this sense:

A sample is analyzed.

An element or compound (analyte) is determined.

Chemical analysis should include a numerical value, and a corresponding unit to indicate the measured quantity, and a statement of uncertainty.^{1,3,4} To determine the composition of unknown samples, measurements often require prior calibration, except for classical methods like gravimetry or titrimetry and absolute instrumental techniques such as coulometry, time-of-flight mass spectrometry (TOF-MS), or isotope ratio mass spectrometry (RMS). Constructing an analytical calibration curve requires adjusting the instrumental range with specific quantities and inputting the concentration of the analyte being measured. Efforts should be made to minimize the uncertainty associated with each measurement, even for techniques that rely solely on injecting a fixed sample volume. Calibration standards for analytical chemistry are typically prepared based on mass fraction rather than volume, as density can vary depending on the dilution solvent. This Letter discusses samples that have already been homogenized in the liquid state and emphasizes the importance of expressing results accurately with appropriate units.

Standardized Units of Measurement: from foundation to actual days

Using a standardized system of units is widely recognized as a valuable tool for effective communication in civil, academic, philosophical, and economic contexts. Expressing scientific data clearly and concisely is essential to ensure comprehension, regardless of the time, region, or country in which the value/unit is

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presented and interpreted.⁵ The International Bureau of Weights and Measures (BIPM) was established in 1875 for the development of unit standardization protocols, promoting consistency in scientific reports. Since then, advances have allowed for even more precise metrics, culminating in the establishment of the seven base quantities/units by the 14th General Conference on Weights and Measures (GCWM) in 1972. These units include the meter for length, the kilogram for mass, the second for time, the ampere for electric current, the Kelvin for thermodynamic temperature, the candela for luminous intensity, and the mole for the amount of substance.

The seven fundamental units of the International System of Units (SI) are insufficient to describe all the events associated with the properties of matter phenomena. When these units are combined, either the same or different, they generate derived units. For example, average velocity (v) is defined as the position variation (meter) per time of the event (second), generating the unit m s^{-1} . Volume (V) is the combination of three spatial dimensions (m), generating the unit m^3 . In some cases, the combining of units results in the creation of derived units with unique names. The SI system currently defines 22 units with notable names, such as the Joule (J), defined as $\text{kg m}^2 \text{s}^{-2}$; the Watt (W), defined as J s^{-1} ; and the Newton (N), defined as kg m s^{-2} .

Furthermore, the metric system is not static and undergoes variations due to new ways of understanding matter, technological advances, or universal constants. For instance, in 2018, the SI unit for mass was redefined because the physical artifact representing the kilogram “lost weight” over 120 years. Thus, the definition of the seven base units is no longer tied to physical artifacts but rather on the fundamental constants of nature. This Letter will focus on the mole and its derivative units, as they are central to expressing data and results in analytical chemistry.

Historically, the mole was defined as the number of atoms in exactly 12 g of carbon-12. However, on May 20, 2019 (World Metrology Day), the GCWM redefined the mole as exactly $6.02214076 \times 10^{23}$ elementary entities, as recommended by the International Union of Pure and Applied Chemistry (IUPAC):

“One mole (mol) contains exactly $6.02214076 \times 10^{23}$ elementary entities. This number is the fixed numerical value of the Avogadro constant, N_A , when expressed in the unit mol^{-1} and is called the Avogadro number. The amount of substance, symbol n , of a system is a measure of the number of specified elementary entities.”^{6,7}

In this sense, the mole (symbol: mol) is the unit for the amount of substance:

“When the mole is used, the elementary entities must be specified and any be atoms, molecules, ions, electrons, other particles, or specified groups of such particles.”⁷

This alteration in the expression of quantities of matter enhances the precision and dependability of measurements. Furthermore, the mole can be directly compared between elements, regardless of their isotopic ratio. While some chemists may require time to adjust to the new scale, the modification should result in more accurate and consistent analytical science.

Chemists typically use molarity (M) to express concentration, which SI defines as the amount of substance (in moles, n) per unit volume (in cubic meter, m^3). Another term, molality, is less commonly used by analytical chemists to express concentration. Molality is defined as the amount of solute entities divided by the mass of the solvent, and according to SI, the formal unit is mol kg^{-1} . Figure 1 shows the correlation between the quantity of matter and mass and how to express concentration using molarity and molality.

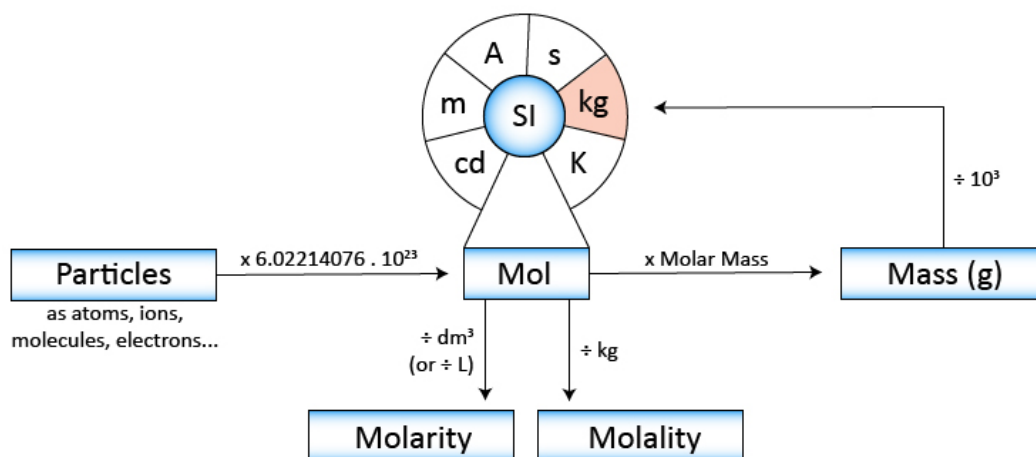


Figure 1. SI units and the centrality of the mole are used to obtain concentrations expressed as molarity or molality.

Common (but unofficial) units

Uniformity in scientific communication is maintained using SI units. However, many units derived from the SI system are dimensionless when analyzing and determining concentrations. For instance, the relationship between the mass of an analyte (in kg) and the mass of a sample (also in kg) is expressed by the unit kg kg^{-1} , which is dimensionless (i.e., equivalent to 1). Similarly, the ratio of moles of product to moles of reagent is represented by mol mol^{-1} , which is also dimensionless. Unofficial units based on ppm, ppb, ppt, etc., are often used, with descriptors based on decimal orders to simplify concentration expression.

Although descriptors such as % (“one part percent”, $1:10^2$), ppm (“one part per million”, $1:10^6$), ppb (“one part per billion”, $1:10^9$), and ppt (“one part per trillion”, $1:10^{12}$) are widely used in laboratories and other areas of chemistry to express low concentrations of substances in solutions, their use is not recommended. These descriptors are not official units and can lead to misinterpretations, especially for non-experts. Analytical chemists must report the results and data concisely, clearly, and reliably. For this purpose, they must adequately equip the informal unit with the correct expression.

Table I displays the relationship between quantities evaluated using official SI units, standard units, and their variations, along with their identification in the form of descriptors. Terms such as “ppm” and “ppb” can have ambiguities because they do not specify whether they refer to parts per million by mass or volume. This ambiguity can lead to confusion and errors in interpreting results, especially when dealing with substances with different densities. Therefore, these terms should not be used whenever possible to express concentrations, especially in a technical report. In many cases, it is beneficial to convert the units to a more widely recognized unit, such as mol L^{-1} (if fraction, $\mu\text{g g}^{-1}$, for instance), to facilitate comparisons between different studies or analyses.

Table I. Official and descriptor units used by analytical chemists to express results

| Quantity | SI Unit | Common units | Variations | Descriptors / informal units | |
|----------------------------|-------------------------|-----------------------|-----------------------|------------------------------|-----|
| | | g g^{-1} (*) | % | - | |
| Mass fraction (ω) | kg kg^{-1} (*) | $\mu\text{g g}^{-1}$ | mg kg^{-1} | g ton^{-1} | ppm |
| | | ng g^{-1} | $\mu\text{g kg}^{-1}$ | mg ton^{-1} | ppb |
| | | pg g^{-1} | ng kg^{-1} | $\mu\text{g ton}^{-1}$ | ppt |

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Table I. Official and descriptor units used by analytical chemists to express results (continued)

| Quantity | SI Unit | Common units | Variations | Descriptors / informal units | |
|---------------------------------|--------------------------------|--------------------------|------------------------|------------------------------|-----|
| Volume fraction (φ) | $\text{m}^3 \text{m}^{-3}$ (*) | L L^{-1} (*) | % | - | - |
| | | mL L^{-1} | $\mu\text{L mL}^{-1}$ | ‰ (= 0.1%) | - |
| | | $\mu\text{L L}^{-1}$ | nL mL^{-1} | - | ppm |
| | | nL L^{-1} | $\rho\text{L mL}^{-1}$ | - | ppb |
| Amount fraction (x) | mol mol^{-1} (*) | mmol mol^{-1} | - | - | - |
| | | $\mu\text{mol mol}^{-1}$ | - | - | - |
| | | nmol mol^{-1} | - | - | - |
| Mass concentration (γ) | kg m^{-3} | g L^{-1} | - | - | - |
| | | mg L^{-1} | $\mu\text{g mL}^{-1}$ | - | ppm |
| | | $\mu\text{g L}^{-1}$ | ng mL^{-1} | - | ppb |
| | | ng L^{-1} | $\rho\text{g mL}^{-1}$ | - | ppt |

(*) are dimensionless quantities or quantities with unit one.

Every analytical chemist has the fundamental ability to convert units to express information as required. However, this task can become problematic if the units are not described correctly, as shown in Table I. To illustrate this, we will consider the practical example of preparing 500 mL of 0.01 mol L^{-1} hydrochloric acid from a 37% m m^{-1} stock (with a density of $\rho = 1.19 \text{ g mL}^{-1}$ at $20 \text{ }^\circ\text{C}$). This task may initially seem complex for students, particularly those in the early stages of their education, due to the need to convert the data.

In this example, the percentage represents a dimensionless mass ratio and, by definition, has no unit (equivalent to 1). However, to achieve the desired molar concentration of 0.01 mol L^{-1} , we can calculate the mass of HCl required (0.1823 g) and the volume (0.4140 mL) of the stock solution (at 37% m m^{-1}), as presented in Box I.

Box I. Calculations were conducted to obtain the theoretical volume value for producing a 0.01 mol L^{-1} HCl solution in 500 mL using 37% m/m solution stock

| | |
|--|---|
| The molar concentration determines the number of moles | $0.01 \text{ mol/L} = \frac{n}{0.5 \text{ L}} \rightarrow n = 5 \cdot 10^{-3} \text{ mol of HCl}$ |
| The mass can be obtained from the number of moles | $n = \frac{m}{\text{MM}} \rightarrow m = (5 \cdot 10^{-3} \text{ mol}) \times \left(36.46 \frac{\text{g}}{\text{mol}}\right) = 0.1823 \text{ g of HCl}$ |
| The total mass of hydrogen chloride in the initial solution | $\rho = \frac{m}{v} \rightarrow m_{\text{total}} = \frac{1.19 \text{ g}}{1.00 \text{ mL}} \cdot \frac{1000 \text{ mL}}{1 \text{ L}} \cdot 1 \text{ L} = 1190 \text{ g}$ $37\% \text{ of } 1190 \text{ g} = 440.3 \text{ g of HCl}$ |
| The volume of the original solution containing the desired mass of acid must be determined | $V = \frac{(0.1823 \text{ g of HCl}) \times (1000 \text{ mL})}{(440.3 \text{ g of HCl})} = 0.4140 \text{ mL}$ |

Table II. Quantities and values were obtained for preparing a 0.01 mol L⁻¹ hydrochloric acid solution from a 37 % m m⁻¹ stock standard ($\rho = 1.19 \text{ g mL}^{-1}$, at 20 °C)

| Quantity | Symbol | Definition | Value | Unit |
|----------------------|-----------------|-------------------------------------|-----------------------|--|
| Mass ratio | $\zeta_{i,j}$ | $\zeta_{i,j} = m_i/m_j$ | $\approx 1 : 2742$ | g g ⁻¹ (*) |
| | ω | $\omega = m_i/\sum m_j$ | 3.65×10^{-4} | g g ⁻¹ (*) |
| Mass fraction | $\omega_{\%}$ | $\omega_{\%} = 100 \times \omega$ | 0.04 | % (*) |
| | ω_{ppm} | $\omega = m_i/\sum m_j$ | 365 | µg g ⁻¹ or ppm (*) |
| Mass concentration | γ | $\gamma = m_i/V$ | 0.365 | g L ⁻¹ , kg m ⁻³ or g dm ⁻³ |
| Volume ratio | $\psi_{i,j}$ | $\psi_{i,j} = V_i/V_j$ | $\approx 1 : 1207$ | mL mL ⁻¹ (*) |
| | φ | $\varphi = V_i/\sum V_j$ | 8.29×10^{-4} | mL mL ⁻¹ (*) |
| Volume fraction | $\varphi_{\%}$ | $\varphi_{\%} = 100 \times \varphi$ | 0.08 | % (*) |
| | φ_{ppm} | $\varphi = V_i/\sum V_j$ | 829 | µL L ⁻¹ or ppm (*) |
| Amount concentration | C | $C = n/V$ | 0.01 | mol L ⁻¹ or mol dm ⁻³ |

In the definitions, m is the mass, V is the volume, and n is the amount of components. (*) are dimensionless quantities or quantities with unit one.

Furthermore, although quantities with volume units ($\psi_{i,j}$, φ , $\varphi_{\%}$, φ_{ppm}) can theoretically be calculated, their use should be avoided due to variations in thermodynamic quantities. Brown (2008) emphasizes the necessity of using units such as mass concentration (γ) and amount concentration (C) along with temperature and pressure conditions.¹ For all chemistry professionals, this argument is fundamental to training and professional development, as effects such as the contraction and expansion of volumes or changes in the density of liquids are frequent in the field. In the field of quality control, verifying the condition of a product or substance is essential for safety. This verification is linked not only to legal regulations but also to the effectiveness of the commercial product. This includes products intended for direct application to the organism, such as medicines and food, as well as those related to quality and stability, and raw material for other processes.

Box II. Calculations were conducted to obtain the values as they apply to chemistry. The quantities used include both official and unofficial units

| | |
|------------------------------|--|
| Mass ratio ($\zeta_{i,j}$) | $\zeta_{i,j} = \frac{0.1823 \text{ g HCl}}{499.8177 \text{ g H}_2\text{O}} = 3.647_3 \cdot 10^{-4} \rightarrow \frac{1}{3.647_3 \cdot 10^{-4}} = 1:2742$ |
| Mass fraction (ω) | $\omega = \frac{0.1823 \text{ g HCl}}{500.00 \text{ g solution}} = 3.646_0 \cdot 10^{-4}$ |

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Box II. Calculations were conducted to obtain the values as they apply to chemistry. The quantities used include both official and unofficial units (continued)

| | |
|-------------------------------------|---|
| Mass fraction ($\omega_{\%}$) | $\omega_{\%} = 100 \cdot (3.646_0 \cdot 10^{-4}) = 0.04 \%$ |
| Mass fraction (ω_{ppm}) | $\omega_{ppm} = \frac{0.1823 \text{ g HCl}}{500.00 \text{ g solution}} \cdot \frac{10^6 \mu\text{g HCl}}{1 \text{ g HCl}} = 365 \mu\text{g g}^{-1} \text{ (ppm)}$ |
| Mass concentration (γ) | $\gamma = \frac{0.1823 \text{ g HCl}}{0.500 \text{ L solution}} = 0.365 \text{ g L}^{-1}$ |
| Volume ratio ($\psi_{i,j}$) | $\varphi = \frac{0.4140 \text{ mL HCl}}{499.586 \text{ mL H}_2\text{O}} = 8.29 \cdot 10^{-4} \rightarrow \frac{1}{8.29 \cdot 10^{-4}} = 1:1207$ |
| Volume fraction (φ) | $\varphi_{\%} = \frac{0.4140 \text{ mL HCl}}{499.586 \text{ mL H}_2\text{O}} = 8.29 \cdot 10^{-4} \text{ mL mL}^{-1}$ |
| Volume fraction ($\varphi_{\%}$) | $\varphi_{\%} = 100 \cdot (8.28 \cdot 10^{-4}) = 0.08 \%$ |
| Volume fraction (φ_{ppm}) | $\varphi_{ppm} = \frac{0.4140 \text{ mL HCl}}{499.586 \text{ mL H}_2\text{O}} \cdot \frac{10^6 \mu\text{L HCl}}{1 \text{ mL HCl}} = 829 \mu\text{L L}^{-1} \text{ (ppm)}$ |
| Amount concentration (C) | $C = \frac{(0.1823 \text{ g HCl})}{(36.46 \text{ g/mol}) \cdot (0.5 \text{ L})} = 0.01 \text{ mol L}^{-1}$ |

Using descriptors as units also poses challenges in environmental management analyses. In Brazil, Resolution 420/2009 from the Brazilian Council for the Environment (CONAMA, 2009) sets criteria and values for soil quality based on the presence of chemical substances in order to assess the impact of human activities on the environment.⁹ According to this resolution, the reference value for lead (Pb) in the soil is 180 mg kg⁻¹. For instance, if a chemical analyst analyzed soil (with density $\rho = 1.4 \text{ g mL}^{-1}$) and obtained a result of 200 ppm, this exceeds the reference value for lead in soil. In this case, since the author omits the unit and presents the answer in the report as a dimensionless descriptor, it can lead to confusion. In this context, if “ppm” corresponds to mg kg⁻¹, the soil would exceed the permitted limit of Pb per kg of soil, indicating anthropogenic activity. Conversely, if “ppm” corresponds to mg L⁻¹, the soil would be within acceptable limits of 143 mg of Pb per kg of soil, signifying no significant human interference. Therefore, the responsibility of a chemical professional extends beyond conducting the analysis and encompasses expressing the results clearly and unambiguously, particularly in sensitive areas such as environmental management.


The provided text briefly discussed the new definition of the mole. Now, the mole is no longer linked to a physical object, the carbon-12 atom, but is defined purely in terms of Avogadro’s constant. In addition to molar concentration, other internationally accepted units and quantities are also presented according to the International System of Units (SI). Some of these units require care in their usage, as they can lead to confusion when used jointly, as is the case with ppm, ppb, and ppt. It is crucial to emphasize that the description of the measured quantity must be clear, precise, and without room for ambiguous interpretations. Accurate communication between the chemical analyst and the requester is essential when presenting a measurement result.

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Maria das Graças Andrade Korn is a Full Professor at the Institute of Chemistry of the University of Bahia (UFBA) with a master's degree in chemistry (Inorganic Analytical Chemistry, 1987) from the Pontifical Catholic University of Rio de Janeiro and a doctorate in chemical sciences from the University of São Paulo (USP) (1997). She was Director of the Analytical Chemistry Division of the Brazilian Chemical Society (2014-2016) and is currently a full member of the Bahia Academy of Sciences. In 2023, she was awarded the Simão Mathias Medal by the Brazilian Chemical Society, and in 2024, the Carol Collins Medal by the SBQ/ENQA Analytical Chemistry

Division for her contribution and scientific prominence in the field of Analytical Chemistry in Brazil. She has always worked in analytical chemistry, developing studies on molecular and atomic spectroscopic techniques and sample preparation procedures applied to different types of food samples, environments, fuels, and medicines. The main focus of her research has been to obtain reliable chemical information through the development of fast methods with improved detectability that are ecologically friendly and mainly target more complex systems in order to meet society's demand. [CV](#)



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