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TUTORIAL

Recommendations on quantities, symbols and measurement units for publications in ACQUAL

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Reporting measurement results in chemistry

For clear and unambiguous reporting of quantitative results it is necessary to follow a set of rules. The recommendations given here are based on internationally agreed rules, in particular on the IUPAC *Compendium of Analytical Nomenclature* (Orange Book, 3rd edn, 1997) and the new edition of *Quantities, Units and Symbols in Physical Chemistry* (IUPAC Green Book, 3rd edn, 2007).

The following quantities are mainly used to report chemical measurement results. These are all quantities used for describing the composition of chemical systems:

mass concentration	$\gamma_{\mathrm{B}} = m_{\mathrm{B}}/V$
mass fraction	$w_{\mathrm{B}} = m_{\mathrm{B}}/\sum m_i$
volume concentration	$\sigma_{\mathrm{B}} = V_{\mathrm{B}}/V$
volume fraction	$\phi_{\mathrm{B}} = V_{\mathrm{B}}/\sum V_i$
amount-of-substance concentration	$c_{\mathrm{B}} = n_{\mathrm{B}}/V$
amount-of-substance fraction	$x_{\mathrm{B}} = n_{\mathrm{B}}/\sum n_i$
amount-of-substance content	$\kappa_{\mathrm{B}} = n_{\mathrm{B}}/m$
molality	$b_{\mathrm{B}} = n_{\mathrm{B}}/m_{\mathrm{A}}$

(m_{A} mass of the solvent).

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V and m denote the total volume and total mass of the mixture. The sums in the denominators of the fractions are the sums over all components of the mixtures prior to mixing, which are equal to the quantities m and n of the mixtures for the mass fraction and the amount-of-substance fraction. In the case of the volume fraction, $\sum V_i$ is, in general, different from V. As the composition of the final mixture is usually of interest, the volume fraction is of minor practical importance. The entities B are either indicated by a subscript or in parentheses, e.g. n_{B} or $n(\mathrm{B})$.

The amount-of-substance content (or amount content) is used mainly in high-accuracy measurement. This quantity and its symbol are not yet included in normative documents. It is, however, a very useful concept, as m is independent of temperature and easy to measure.

The most important general rules for the use of quantities and units

SI units are used throughout except where non-SI units are more common, e.g. 'litre'.

The symbols of quantities are written in italics, those of units in roman. Subscripts, which represent quantities including running variables such as i, j, k are written in italics, but in roman if they represent labels, e.g. n_{B} for the entity B.

Products of units require a space (or ·) between the units. Prefixes are directly combined with units, e.g. mmol, μL. The combination is taken as a new symbol that can be raised to any power without the use of parentheses, e.g. mmol^{-1}.

Examples of reports of chemical measurement results

The measurement uncertainty, which is part of the measurement result, is not included here in the result.

(a) The mass concentration of lead in the waste water sample is
$\gamma(\mathrm{Pb})$ = 12.8 mg/L (= 12.8 mg L^{-1} = 12.8 g/m^3 = 12.8 g m^{-3} = 0.0128 g/L).

For the volume unit 'litre' both l and L are used. The lower case letter has the disadvantage that it can easily be confused with the figure one. Therefore L is preferred.

(b) The mass fraction of sulphur in the coal sample is
$w(\mathrm{S})$ = 0.0078 (= 0.0078 g/g = 7.8 mg/g = 7.8 g/kg = 7.8 g kg^{-1}).

Combinations like 7.8 mg S/g coal are not acceptable.

(c) The volume concentration of ethanol in the wine sample is
σ = 135 mL/L.

On wine bottle labels notations like '13.5% vol' are used. This is not recommended for reporting chemical measurement results.

(d) The amount-of-substance concentration (or concentration) of cholesterol in the human serum sample is
c = 5.31 mmol/L (= 5.31×10^{-3} mol/L = 5.31 mol m^{-3}).

In clinical measurement and medical practice mass concentration in mg/dL is often used, which is also acceptable. In solution chemistry (e.g. titrimetry) expressions like: 0.1 M HCl (M for mol/L) are sometimes used. This is not encouraged. Instead, $c(\mathrm{HCl})$ = 0.1 mol/L should be used.

(e) The amount-of-substance fraction of CO_2 in the calibration gas mixture is
$x(\mathrm{CO_2})$ = 422 µmol/mol (= 422×10^{-6}).

The notations 'ppm' for 10^{-6} and '%' for 10^{-2} are not encouraged, but may be acceptable when there is no doubt about the unit used. Combinations with quantities like 'ppmv' or '%(m/m)' are not acceptable.

(f) The amount-of-substance content (or amount content) of Cd in a natural water sample is
$\kappa(\mathrm{Cd})$ = 82.38 nmol/kg.

(g) The molality of Na_2HPO_4 in the buffer solution is
$b(\mathrm{Na_2HPO_4})$ = 0.03043 mol/kg.

Additional remarks on some quantities not appearing in the IUPAC Green Book, 3rd edn

The quantity 'volume concentration', symbol σ, is not defined in the Green Book, but is taken from DIN 1310 and T. Cvitaš (1996) Metrologia, 33:35–39. The quantity 'amount content' is also not included in the Green Book. It was also taken from T. Cvitaš (same reference). Instead of k, the symbol κ is used to avoid confusion with the coverage factor k. Both quantities are important in chemical measurement.