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INTERUNION COMMISSION ON BIOTHERMODYNAMICS*

RECOMMENDATIONS FOR THE PRESENTATION OF THERMODYNAMIC AND RELATED DATA IN BIOLOGY

(Recommendations 1985)

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Recommendations for the presentation of thermodynamic and related data in biology

(Recommendations 1985)

Abstract

Thermodynamic data are important in describing and in developing an understanding of biological systems. However, at present there is a marked variation in the terminology and symbols used in this connection. A guide has been prepared in which SI units and symbols of special importance for biothermodynamics are summarized together with examples and with comments concerning their use. It is recognized that in some cases recommendations made by IUPAC may have to be adjusted slightly or developed further in order to suit the practical needs in the biological sciences. In the present report suggestions are given with this purpose in mind.

The overall aim of the report has been to prepare a document which will serve as a practically useful guide for those who are involved in scientific writing and in teaching in the field of biothermodynamics. The document is therefore intended to be largely self-contained.

Physicochemical data are of considerable importance in describing and in developing an understanding of biological systems. At present, there is marked variation in the terminology and symbols used for physicochemical quantities and in the units of measurement in which they are reported in the biological literature. This situation leads to confusion and many difficulties in comparing and correlating the results from different laboratories. Recommendations concerning units, symbols and terminology have been made by the international standardizing bodies in order to facilitate communication and to remove ambiguities. These recommendations emphasize the use of the modern metric system of units called the Système International (SI) d'Unités (International System of Units) [1], which differs in several important ways from previous scientific usage.

Such recommendations cannot always be expected to be immediately accepted and used in all fields. It is hoped that the present transition period can be made as short as possible and that future generations of scientists will not be unnecessarily burdened by the variety of units and symbols currently found in textbooks, research reports and data compilations. We therefore encourage scientists studying biological systems to accept and to use the SI whenever suitable.

In this document, SI units and symbols of special importance for biological sciences and their applications to particular quantities are summarized. A more complete discussion of the SI, together with recommendations for symbols and terminology used to describe quantities of importance in physical chemistry is given in IUPAC's 'Manual of symbols and terminology for physicochemical quantities and units' [2] and also [3]. For other discussions of the presentation of numerical data and of thermodynamic data derived from experiments, we call attention to guides prepared by CODATA [4] and IUPAC [5].

Although we believe it is important to avoid differences in terminology and symbols in physical chemistry and in the biological sciences, we realize that some recommendations made by IUPAC may have to be adjusted or further developed in order to suit the practical needs in the biological sciences. In the present document, some recommendations are given with this purpose in mind.

The Interunion Commission on Biothermodynamics has previously made recommendations for terminology in two special areas of biothermodynamics: 'Recommendations for presentation of biochemical equilibrium data' [6] and 'Calorimetric measurements on cellular systems. Recommendations for measurements and presentation of results' [7]. In order to facilitate the practical use of the recommendations, they have been prepared to be largely self-contained. There is thus some unavoidable overlap between the present and previous documents.

PHYSICAL QUANTITIES, SI UNITS AND THEIR SYMBOLS

A physical quantity is the product of a numerical value (a pure number) and a unit. By international agreement a set of seven dimensionally independent units form the so-called SI base units [1 – 3]. The base physical quantities and units and their recommended symbols are summarized in Table 1.

The symbols for physical quantities should be printed in italic (sloping) type of the Latin or Greek alphabets or underlined in typescript, and the symbols for units should be printed in roman (upright) type.

Table 1. *SI base quantities and units*

Base quantities		Base units	
Name	symbol	name	symbol
Length	l	metre	m
Mass	m	kilogram	kg
Time	t	second	s
Electric current	I	ampere	A
Temperature*	T	kelvin	K
Amount of substance	n	mole	mol
Luminous intensity	I_v	candela	cd

* Thermodynamic ('absolute') temperature. Recommended symbol for Celsius temperature is t or θ. Where symbols are needed to represent both time and Celsius temperature, t is the preferred symbol for time and θ for Celsius temperature [2].

All other physical quantities and units are regarded as being derived from the base quantities and units. Certain SI-derived units have been given special names and symbols. In Table 2, symbols and units for some thermodynamic quantities (functions) are given. For more complete tabulations of quantities and units recommended for chemistry and physics, see [2, 3].

The SI base units are often cumbersome to use in practical work and therefore the use of certain prefixes denoting multiples or submultiples is convenient. Recommended prefixes are listed in Table 3.

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Table 2. *Symbols and units for some thermodynamic quantities*

Quantity		SI unit	
Name	symbol	name	symbol
Volume	V	cubic metre	$\mathrm{m^3}$
Force	F	newton	$\mathrm{N = m\,kg\,s^{-2}}$
Density	ϱ	kilogram per cubic metre	$\mathrm{kg\,m^{-3}}$
Pressure	p	pascal	$\mathrm{Pa = N\,m^{-2}}$
Viscosity	η	pascal second	$\mathrm{Pa\,s}$
Energy	E	joule	$\mathrm{J = N\,m}$
heat	q, Q*	joule	$\mathrm{J = N\,m}$
work	w, W*	joule	$\mathrm{J = N\,m}$
internal energy	U, (E)	joule	$\mathrm{J = N\,m}$
enthalpy: $U + pV$	H	joule	$\mathrm{J = N\,m}$
Gibbs energy: $H - TS$	G	joule	$\mathrm{J = N\,m}$
Helmholtz energy: $U - TS$	A	joule	$\mathrm{J = N\,m}$
Entropy	S	joule per kelvin	$\mathrm{J\,K^{-1}}$
Power	P	watt	$\mathrm{W = J\,s^{-1}}$
Heat capacity			
at constant pressure: $(\delta H/\delta T)_p$	C_p	joule per kelvin	$\mathrm{J\,K^{-1}}$
at constant volume: $(\delta U/\delta T)_V$	C_V	joule per kelvin	$\mathrm{J\,K^{-1}}$
Cubic expansion coefficient: $V^{-1}(\delta V/\delta T)_p$	α	per kelvin	$\mathrm{K^{-1}}$
Isothermal compressibility: $-V^{-1}(\delta V/\delta p)_T$	κ	per pascal	$\mathrm{Pa^{-1}}$
Osmotic pressure	Π	pascal	Pa
Chemical potential of substance B	μ_B	joule per mole	$\mathrm{J\,mol^{-1}}$
Absolute activity of substance B	λ_B	dimensionless	
Relative activity of substance B	a_B	dimensionless	
Activity coefficient, mole fraction basis	f_B	dimensionless	
Activity coefficient, molality basis	γ_B	dimensionless	
Activity coefficient, concentration basis	y_B	dimensionless	
Osmotic coefficient	ϕ	dimensionless	

* It is recommended that $q > 0$ and $w > 0$ both indicate increases in the energy of the system under discussion [2]. Thus $\Delta U = q + w$.

Table 3. *SI prefixes*

Multiplier	Prefix	Symbol	Multiplier	Prefix	Symbol
10^{-1}	deci	d	10	deca	da
10^{-2}	centi	c	10^{2}	hecto	h
10^{-3}	milli	m	10^{3}	kilo	k
10^{-6}	micro	μ	10^{6}	mega	M
10^{-9}	nano	n	10^{9}	giga	G
10^{-12}	pico	p	10^{12}	tera	T
10^{-15}	femto	f	10^{15}	peta	P
10^{-18}	atto	a	10^{18}	exa	E

SOME COMMENTS CONCERNING CHOICE OF UNITS IN BIOTHERMODYNAMICS

Mass: specific and molar quantities

The SI base unit of mass is the kilogram. However, its multiples and submultiples are named and symbolized as multiples and submultiples of the gram. *Example:* μg, not nkg for 10^{-9} kg.

The term 'specific' preceding the name of an extensive quantity means 'divided by mass' and the specific quantity should preferably be designated by a lower case letter. (An 'extensive' physical quantity for a system depends on the amount of material it contains.) *Example:* c_p is the specific heat capacity at constant pressure. A suitable unit is $\mathrm{J\,K^{-1}\,g^{-1}}$. (The term 'specific heat' is an inappropriate term for specific heat capacity.)

The term 'molar' preceding the name of an extensive quantity means 'divided by amount of substance', giving, in effect, the quantity per mole. The quantity should be represented by a capital letter and the attached lower case subscript, m. *Example:* $C_{p,\mathrm{m}}$ is the molar heat capacity ($\mathrm{J\,K^{-1}\,mol^{-1}}$) at constant pressure. The subscript, m, can be omitted when there is no risk of ambiguity.

Thermodynamic quantities should, where possible, be reported in terms of molar quantities. For biochemical macromolecules the molecular mass (dalton, a non-SI unit of mass, symbol Da) or, the numerically identical, molar mass ($\mathrm{g\,mol^{-1}}$) used in the calculations should always be reported (cf. [8]). If the quantity of a substance is determined by weighing, the water content and other known or estimated impurities should be reported and corrections applied. In cases where the molecular mass is not known, the amount of compound should, where possible, be reported in an SI mass unit.

Volume

The SI unit for volume is the cubic metre ($\mathrm{m^3}$). More convenient units in biothermodynamics are usually its submultiples: cubic decimetre ($\mathrm{dm^3}$), cubic centimetre ($\mathrm{cm^3}$) and cubic millimetre ($\mathrm{mm^3}$). The symbol 'cc' (to denote $\mathrm{cm^3}$) should not be used.

The cubic decimetre is identical to the litre (l or L). This non-SI unit and its submultiples, the millilitre ($1\ \mathrm{ml} \equiv 1\ \mathrm{cm^3}$), the microlitre ($1\ \mu\mathrm{l} \equiv 1\ \mathrm{mm^3}$), and the nanolitre ($1\ \mathrm{nl} \equiv 10^{-12}\ \mathrm{m^3}$) are in biology often considered to be more convenient and more readily understood than corresponding SI units. One can therefore expect the litre-based volume units to be used alongside the SI units (cf., however, comments under *Pressure*).

Time

The SI base unit for time is the second (s). Other units for time which are exactly defined in terms of the second are the minute (min, not mn), hour (h, not hr), and day (d). However, when reporting measured values of properties involving time, the use of min, h and d is discouraged. It should be realized that the second, or its multiples or submultiples, is employed as the basic unit of time in most electronic instruments used for determination of time-dependent physical quantities. Furthermore, power in watts is obtained directly by dividing energy in joules by time in seconds.

Temperature

Thermodynamic temperatures and temperature differences are expressed in the SI base unit, the kelvin, symbol K (not degrees Kelvin or °K). Temperature and temperature differences may also be expressed in degrees Celsius, symbol °C. The degree Celsius was formerly called the degree 'centigrade'. To many biologists the Celsius scale is more convenient to use, e.g. to express an experimental temperature. However, it is recommended that whenever values for temperatures are used in connection with thermodynamic calculations, they are reported in kelvins.

Pressure

The SI unit of pressure is the pascal, which is one newton per square metre ($\mathrm{Pa} = \mathrm{N\,m^{-2}}$). A convenient unit for many pressure measurements is the kilopascal (symbol kPa). The biological thermodynamicist should recognize that the common thermodynamic term, pV, is an energy term, and if p is in pascals and V is in cubic metres, then the pV product is obtained directly in joules. Note that combinations of customary non-SI units all require the use of a conversion factor.

The commonly found units mmHg or Torr are exactly defined in terms of Pa but should be avoided (cf. [2]).

One atmosphere is defined as 101 325 pascals (1 atm = 101.325 kPa). However, the atmosphere is a non-SI unit and its use should be avoided. The IUPAC Commission on Thermodynamics has recently recommended that 10^5 Pa (1 bar) be adopted as the standard state pressure in chemical thermodynamics [9]. In calculating equilibrium constants and standard thermodynamic functions based on pressure measurements, it should be recognized, however, that the accepted standard state pressure for many years has been 1 atmosphere.

Viscosity

The SI unit for viscosity (η) is the pascal-second ($\mathrm{Pa\,s} = \mathrm{kg\,s^{-1}\,m^{-1}}$). Traditionally used non-SI units are the poise (P) or the centipoise (cP), 1 Pa s being equal to 10 P.

Energy

Energy measurements, including all thermal measurements, should be reported in joules (J), kilojoules (kJ) or millijoules (mJ) as appropriate. The use of 'calorie' is discouraged (cf. [7]). The 'thermochemical calorie' ($\mathrm{cal_{th}}$) is defined as $1\ \mathrm{cal_{th}} \equiv 4.184\ \mathrm{J}$.

Entropy

The recommended SI unit is joule per kelvin ($\mathrm{J\,K^{-1}}$). The use of 'entropy units' ('e.u.') is not acceptable.

Power

The SI unit of power is watt (W). More convenient units in biothermodynamics are usually milliwatt (mW), microwatt (μW), picowatt (pW) or femtowatt (fW). The use of units such as calories per hour, which is currently common in biology, is discouraged (cf. [6]).

Density

The SI for density (ϱ) is $\mathrm{kg\,m^{-3}}$. A more convenient unit is usually $\mathrm{g\,cm^{-3}}$.

NOTATIONS FOR VARIABLES, STATES AND PROCESSES

Variables

Variable parameters for the thermodynamic functions can be indicated in parentheses after the symbols, e.g. $C_p(T,p)$.

Table 4. *Some recommended superscripts*

Superscript	Meaning
$\ominus$ (or $\ominus$)	standard
*	pure substance
∞	infinite dilution
id	ideal
$'$	apparent (cf. the text)
E	excess
$\ddagger$	activated complex

Table 5. *Symbols for states of aggregation*

State	Symbol
Gas	g
Liquid	l
Solid	s
Fluid	fl
Liquid crystal	lc
Crystalline solid	cr
Amorphous solid	am
Vitreous substance	vit
Solution	sln
Aqueous solution	aq

Similarly, values for quantities can be represented by an appropriate symbol with values for the established conditions given in parentheses. *Example:* C_p (298.2 K, 0.1 MPa, pH = 7.0) or C_p (25.0°C, 1 bar, pH = 7.0).

States

Superscripts to symbols for properties (thermodynamic functions) are frequently used to denote a particular state (Table 4). *Example:* $C^*_{p,\mathrm{B}}$ is the (molar) heat capacity for the pure substance B at constant pressure.

The term 'apparent' indicated by a superscript $'$ is used to mean that a process is not well known or that its value carries uncertainties which are not known. *Example:* $\Delta G^{0\prime}$ is the apparent standard Gibbs energy change. For a detailed discussion of K′ (apparent equilibrium constant) and $\Delta G^{0\prime}$, see [6].

The word 'apparent' is used in a different sense in the context of partial molar quantities. As a symbol for 'apparent' in this connection, the use of subscript ϕ, as in Y_ϕ, is recommended. Other notations employed for this property include ${}^{\phi}X$ and ϕ_X. *Example:* The apparent molar volume V_B of a solute B is defined by $V_{\mathrm{B},\phi} = (V - n_\mathrm{A} V^*_\mathrm{A})/n_\mathrm{B}$, where n_A and n_B are the amounts of solvent and solute, respectively. V is the total volume of the solution and V^*_A is the molar volume of the pure substance A.

To denote a state of aggregation it is recommended that an appropriate symbol be given in parentheses after the symbol for the thermodynamic quantity. The symbols given in Table 5 have recently been recommended by the IUPAC Commission on Thermodynamics [9]. *Example:* $V^*_\mathrm{B}(\mathrm{cr})$ is the (molar) volume of substance B in its pure crystalline state (cf. Table 5).

It is not practical to give definite recommendations for symbols for all states which are of relevance in biological systems. In many cases the terms used, for example 'helix' and 'coil', imply structural knowledge which is only presumed. In other cases the terms used, for example 'native' and 'denatured', are strictly operational and their meanings vary from situation to situation. Therefore it is urged that when such terms are used they be well defined within the context of their use and that their associated symbolic representation be judiciously selected. Any such notation should be used with caution and in all cases the text should clearly describe the state to which a value or function refers.

Processes

A thermodynamic change is denoted by the symbol Δ before the corresponding quantity. The nature of the change is signified by annotation of the Δ. Two methods of annotation are now recommended by the IUPAC Commission on Thermodynamics [9]:

i) use of regular symbols as superscripts and subscripts: the notation $\Delta_\alpha^\beta X$ is recommended to denote the change in property X for the process $\alpha \rightarrow \beta$ where α and β are symbols for states or species. *Example:* $\Delta_s^l H$ meaning the change in enthalpy when a substance changes from the solid to the liquid state.

ii) use of special subscripts to denote the process. The subscript symbols given in Table 6 have been recommended [9]. *Example:* $\Delta_c S_B$, meaning the entropy of combustion of substance B.

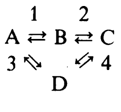
Currently the symbol for a process is usually placed as subscript to the symbol for the property, e.g. ΔS_c. This practice is likely to prevail for some time in biothermodynamics.

For many processes of biological relevance, the symbols listed in Table 6 are insufficient. In those cases, for example ionization, protonation and oxidation, the process should be well defined in the text and the symbol used should be judiciously selected.

Table 6. *Symbols for processes*

Process	Symbol (subscript)
Vaporization (evaporation)	vap
Sublimation (evaporation)	sub
Melting (fusion)	fus
Transition of one solid phase to another	trs
Mixing of fluids	mix
Solution (dissolution)	sol
Reaction (except for combustion)	r
Combustion	c
Formation (of a component from its elements)	f

It should be realized that in biochemical thermodynamics processes are not always well defined. Rather than using special symbols it is therefore often advisable to use 'neutral' symbols like a, b, . . . or 1, 2, . . ., which should be clearly identified in the text. In cases where one is dealing with complex reaction schemes, these should always be represented by a figure in the text. It is then recommended that each reaction step be given a 'neutral' symbol. *Example:*



SOLUTIONS

The word 'solution' is used to describe a liquid or solid phase containing more than one component. For convenience one of these substances is referred to as 'solvent' (normally the one present in the largest concentration) and all others as 'solutes'. In biological solutions, which generally contain a number of components, the distinction is not always clear and often a fixed mixture of components is referred to as 'solvent' (e.g. H_2O plus buffer components), with all other substances being defined 'solutes'.

Recommended notations for composition of solutions are summarized in Table 7.

Subscript A (or 1) is sometimes used to denote the solvent and B (or 2) the solute, but the designation of subscripts should always be defined.

A convenient unit of concentration, sometimes called 'molarity', is mol dm^{-3}. A solution with a concentration of 0.1 mol dm^{-3} is often called a 0.1 molar solution or a 0.1 M solution. Because the term molarity and the symbol M are liable to be confused with molality (Table 7), the term 'concentration' and the symbol 'mol dm^{-3} (mol l^{-1}, mol L^{-1})' are preferred.

In the particular case of aqueous solutions, the solvent can be denoted by 'aq', but usually not by 'H_2O'. The latter notation should only be used for pure water or, possibly, in cases where presence of solutes is insignificant for the problem considered.

Authors should be aware of the fact that concentrations of low-molecular-weight components diffusible through semi-permeable membranes in solutions of biological macromolecules prepared by equilibrium dialysis may differ from the concentrations of these solutes in the dialysis solvent. The chemical potentials, μ, of the diffusible solutes, though, are identical in both the macromolecular solution and in the dialysis solvent. The composition of the dialysis solvent should therefore be stated precisely (cf. [10, 11]).

A partial molar quantity of substance B is defined as $Y_B = (\delta Y / \delta n_B)_{T, p, n_C \ldots}$ where Y is an extensive quantity of a system. *Examples:* $V_B = (\delta V / \delta n_B)_{T, p, n_C \ldots}$, the partial molar volume of substance B; $v_B = (\delta v / \delta m_B)_{T, p, m_C \ldots}$, the partial specific volume of substrate B.

If the partial quantity refers to infinite dilution, it should be so designated by the superscript symbol $^{\infty}$ (cf. Table 4).

The symbol $\bar{Y}_B$ is often used instead of the recommended Y_B. The bar over Y resolves no ambiguity; in fact, it is misleading, as the bar is often used to indicate an average (cf. [3]).

The condition to which an apparent molar quantity, Y_ϕ, refers should be clearly stated in the text or indicated in the symbol. *Example:* $V_{B,\phi}$(aq, c = 0.1 mol dm^{-3}), meaning the apparent molar volume of substance B in aqueous solution where the concentration of B is 0.1 mol dm^{-3}.

Table 7. *Notations for composition of solutions*

Quantity		Practical unit
Name	symbol	
Amount of substance B	n_B	mol
Concentration of solute substance B (the amount of substance of B divided by the volume of the solution)	c_B, [B]	mol dm^{-3}
Mass concentration of substance B (mass of B divided by the volume of the solution)	ϱ_B	g dm^{-3}
Molality of solute substance B (the amount of substance of B divided by mass of principal solvent)	m_B	mol kg^{-1}
Mole fraction of substance B ($n_B/\Sigma_J n_J$)	x_B	dimensionless
Mass fraction of substance B ($m_B/\Sigma_J m_J$)	w_B	dimensionless
Volume fraction of substance B ($V_B/\Sigma_J V_J$)	ϕ_B	dimensionless

PRESENTATION OF RESULTS

Whenever values for quantities are reported – in a text, a table, a graph or in a projected slide – the units should also be given. In addition, necessary information concerning vital experimental parameters (temperature, concentration, pH, solvent composition, etc.) should be stated. It is not always practicable to include adequate experimental parameters in the table or graph itself, or even in the accompanying legend. The necessary additional information must then be given in the text.

When thermodynamic results are given in a table, it is usually most convenient to list them as pure numbers with the unit given in the table legend or preferably in the columnar heading. It is then correct to give the symbol for the quantity divided by the symbol for the unit. *Example:* $\Delta H/(\mathrm{kJ\ mol^{-1}})$ or $\frac{\Delta H}{\mathrm{kJ\ mol^{-1}}}$, meaning that the numbers reported in the table are enthalpy changes expressed in the unit kilojoule per mole.

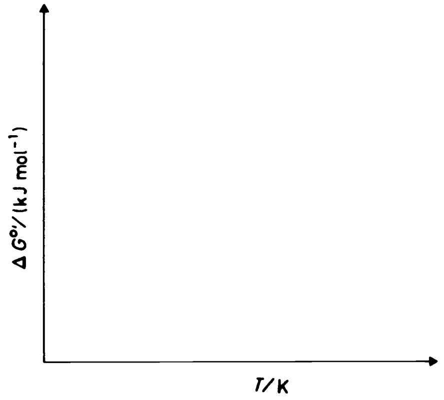


Fig. 1. *Apparent standard Gibbs energy change expressed in kilojoules per mole, as a function of temperature, given in kelvins*

The axes of graphs and the headings in tables should be labeled with both the name (or symbol) of the quantity and the unit employed so as to give a dimensionless ratio for plotting or tabulation. An example of this is given in Fig. 1.

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