Units and Dimensions in Physical Chemistry

Units and dimensions tend to cause untold amounts of grief to many chemists throughout the course of their degree. My hope is that by having a dedicated tutorial on them we can avoid this for Hertford chemists. It is very important that you understand everything in this tutorial and that you (eventually) find the associated problems quite straightforward. Please make sure you ask lots of questions if there are things you don't understand (this goes for all tutorials, of course).

SECTION A – Reading and notes

Read the material taken from the book 'Quantities, units and symbols in physical chemistry' (often called the 'Green Book'), and also the overview below. Read them in any order you like, and take notes if it helps you.

Physical quantitites

A physical quantity is the product of a numerical value and a unit.

(Physical quantity) = (numerical value) x (unit)

e.g. (mass of an average person) = (70) x (kg) Obviously, this is usually just written 70 kg.
(speed of light) = (2.99792458×10^{8}) x (ms^{-1})

If you are one of the many people who, up until now, has always thought of units as something you have to tack onto the end of your calculations, appreciating the significance of the above is even more important. In science, we are generally dealing with physical quantities, not with pure numbers (we'll leave that to the mathematicians). This means that virtually every number you write down should have units with it. The numerical value of a physical quantity will vary depending on what units you choose to use (for example, an energy of 1 kJ could equally well be expressed as 1000 J, or 6.242×10^{21} eV, or 2.294×10^{20} Hartree), which means that just writing down a number without also stating its units is completely meaningless. *Units are not optional!*

The good news is that by thinking of units in this way, all the calculations and conversions and conventions that you previously may have found tortuous and completely incomprehensible should suddenly become much more straightforward. All calculations to do with units now essentially just become very basic algebra. For example, the tick marks along the axis of a graph are generally only labelled with numerical values. The axis label must therefore be consistent with this. Rearranging the above equation gives (numerical value) = (physical quantity)/(unit), so axes should always be labelled to be consistent with this e.g. speed / ms^{-1}, or mass / kg. The alternative, often seen in publications from the US and written e.g. speed (ms) or mass (kg) is technically incorrect and unfortunately shows that the authors do not understand physical quantities.

Before we move onto calculations, we need a short recap of the SI (Système Internationale) system of units.

SI units

The SI system identifies base units. These are defined very precisely (see the Green Book material for details) and are independent of one another.

Quantity	Unit	Symbol
Mass	kilogram	kg
Length	metre	m
Time	second	s
Current	Ampere	A
Temperature	Kelvin	K
Amount	mole	mol

All other SI units can be expressed in terms of these base units. You can work out the definitions very easily if you know a definition of the quantity you're interested in.

For example, the SI unit of energy is the Joule (J). If we want to know how a Joule is defined in terms of the base units, we could use the definition of the kinetic energy of a moving object:

$E = \frac{1}{2} mv^2$, where m and v are the mass and velocity of the object.

You will be used to substituting numerical values into this type of equation, but really what you are doing is substituting in *physical quantities*. The only reason you don't usually substitute in the units with your numerical value is that the units part of the calculation is the same every time, so you already know the result (though you may not have realised this before!). Consider the kinetic energy of a 10 kg object travelling at 2 $\mathrm{ms^{-1}}$.

$$\mathrm{E = \tfrac{1}{2}\,(10\ kg)(2\ ms^{-1})^2 = 40\ kg\ m^2\ s^{-2} = 40\ J}$$

We see that the units of J are equivalent to kg $\mathrm{m^2\ s^{-2}}$. If we're *just* interested in relationships between units, then we can just substitute the units into an equation (just as if we're just interested in the numerical result then we only substitute the numerical values into an equation). If we're just doing a units calculation then we can ignore constant factors (e.g. the factor of ½ in the equation for the kinetic energy).

As another example, consider the potential energy of an object in the gravitational field of the earth at a height h above the earth's surface.

$E = mgh$, where g is the acceleration due to gravity, 9.8 $\mathrm{ms^{-2}}$.

A units calculation would therefore give:

$$\mathrm{J = (kg)\ (ms^{-2})\ (m) = kg\ m^2\ s^{-2}.}$$

Reassuringly, this is the same result as before. Hopefully this convinces you that you can choose any equation you like to work out how to express an SI unit in terms of the base units.

Often, you will see SI units with prefixes, which denote powers of ten. You need to know these prefixes (at least up to powers of plus or minus 15).

10^{-1}	deci	d	10^{1}	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
10^{-21}	zepto	z	10^{21}	zetta	Z
10^{-24}	yocto	y	10^{24}	yotta	Y

Calculations with physical quantities

There are a few very simple rules regarding calculations with physical quantities.

1. You can only add or subtract quantities with the same units e.g. 10 kg + 5 kg = 15 kg, while 10 kg + 400 m is completely nonsensical. Note: check that you have all energies in the same units before carrying out this type of calculation e.g. all in J or all in kJ, not a mixture of the two.

2. When you multiply or divide, the units multiply and divide with the quantities, as shown in the previous section.

3. The arguments of logs, exponentials, and other functions that may be expanded as power series may only be dimensionless numbers.

   e.g. $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}$

   If x was not dimensionless, every term in the expansion would have different units!

   This can be very useful in helping us work out the units of physical quantities. For example, a first order radioactive decay can be described by the equation $n = n_0 e^{-kt}$, where n is the amount of substance, n_0 is the amount of substance at time zero, k is the rate constant for the decay, and t is time. If we didn't know the units for the rate constant, we could use the fact that the product kt must be dimensionless to work them out. Since we know that time has units of seconds, k must have units of s^{-1}.

Unit conversions

This is an area in which many students frequently get themselves in a complete tangle or despair completely. However, once you have the definition of a physical quantity clear in your head it is really very simple to convert between units.

As an example, consider the volume V of a cube with sides of length L.

$$V = L^3$$

In SI units, L would be given in m, and V would therefore be in m^3. Assume we have sides of length 2 m. This would give a volume of 8 m^3. However, what if we wanted to know the volume in cm^3? Simple: 1 m = 100 cm, so:

$$V = (2\ m)^3 = (2 \times 100\ cm)^3 = 8\times10^6\ cm^3$$

Consider a second example. Suppose we want to convert 324 kJ mol^{-1} into J $molecule^{-1}$. We know that 1 kJ = 1000 J, and that 1 mol = 6.022×10^{23} molecules. Therefore:

$$324 \text{ kJ mol}^{-1} = 324 \times (1000 \text{ J}) \times (6.022 \times 10^{23} \text{ molecules})^{-1} = 5.38 \times 10^{-19} \text{ J molecule}^{-1}$$

Dimensional analysis

Sometimes we can work out the form of an equation simply by knowing the units of the quantities involved. There is often only one combination of the quantities that is consistent with their units. As a very simple example, suppose somebody tells you that the speed of an object has units of ms^{-1}, and they know that you can work out the speed of an object from the distance it has travelled and the time it took to travel that distance. However, they can't remember the required equation. You can work it out by looking at the units:

Speed v has units of ms^{-1}
Distance d has units of m
Time t has units of s

The obvious combination of quantities with units of m and s to give a quantity with units of ms^{-1} is

$$v = d / t$$

We could have done this calculation in a more formal way by equating powers of units i.e.

$$(\text{speed}) = (\text{distance})^a \, (\text{time})^b$$

So in terms of units $\quad (ms^{-1}) = (m)^a \, (s)^b$

We immediately see that a = 1 and b = -1, so speed = $(\text{distance})^1(\text{time})^{-1}$, or $v = d / t$ as before.

We can also go back to our kinetic energy example. Suppose you know that kinetic energy is measured in J (and that the equivalent in SI base units is kg m^2 s^{-2}, and you also know that the kinetic energy depends on the mass of the object and on its velocity, but you can't remember the relationship.

$$(\text{Energy}) = (\text{mass})^a \, (\text{velocity})^b$$

So in terms of units $\quad (kg\ m^2\ s^{-2}) = (kg)^a \, (ms^{-1})^b$

It is very straightforward to see that a = 1 and b = 2. If it had been less straightforward we could have matched terms on the left and right hand sides of the equation

$$kg = kg^a$$
$$m^2 = m^b$$
$$s^{-2} = (s^{-1})^b$$

which again gives a = 1, b = 2. Our dimensional analysis therefore tells us that

$$E \propto mv^2$$

Dimensional analysis unfortunately can only give us the proportionalities between physical quantities. In this case it cannot give us the required factor of ½.

SECTION B – Problems

1. Identify the SI units for the following quantities, and use the accompanying expressions to express them in terms of SI base units.

   (a) Force $F = ma$, where F = force, m = mass, a = acceleration

   (b) Pressure $p = F/A$ where p = pressure, F = force, A = area

2. How many dm^3 are there in one m^3?

3. When a substance diffuses, the *flux* is defined as the rate at which the amount of substance diffuses per unit area. According to Fick's law of diffusion, the flux is equal to minus the diffusion coefficient, D, times the concentration gradient, dc/dx.

   (a) What are the correct SI units for the flux and the concentration gradient?

   (b) Hence deduce the SI units for the diffusion coefficient.

4. The universal gas constant, R, can be calculated from measurements of pressure, volume, temperature and amount of substance under ideal conditions from $R = pV/nT$.

   (a) Find the SI units for R.

   (b) 1 mol of gas occupies 24.8 m^3 at 298 K and 1.00 mbar. Calculate R.

   (c) What is the concentration of the gas? (mol dm^{-3} and molecules cm^{-3}).

5. Consider the following statement:

   "It is not permitted to take the log of a unit, so in the equation $\Delta G^{\ominus} = -RT \ln K$, the equilibrium constant has no units. The only equilibrium constants with no units are for equilibria with equal numbers of particles on each side of the reaction equation, and so the equation above is only meaningful for reactions of this type."

   Which of the following is the best statement of the flaw in this argument?

   A Units are always ignored when logarithms are taken.
   B The units of K depend on the relative numbers of reactants and products in the chemical equation.
   C In calculating K, it is necessary to use activities instead of concentrations, and activities are dimensionless.
   D There is no flaw in this argument.

6. A molecule of carbon dioxide occupies a volume of 3.2×10^{-26} m^3. In the British system the smallest unit of volume is the minim, which is equivalent to 0.05919385 cm^3. What is the volume of the molecule in minims?

7. The speed limit on a road in Rutland is 135000 furlongs per fortnight. Given that a furlong is 1/8 mile and a fortnight is 14 days, calculate the speed limit in miles per hour.

8. The slug is an American unit of mass equivalent to 14.5939 kg, and 1 foot = 30.48 cm (exactly). The density of a soil sample is 3.01 g cm^{-3}. Convert this density to slugs per cubic foot.

9. A solution of sodium chloride has concentration 0.15 mol dm^{-3}. Convert this concentration into molecules nm^{-3}.

10. (a) Express the SI units for density and pressure in terms of SI base units.

    (b) Gas escapes through a small hole in the side of a vessel. The rate of loss of mass depends on the pressure of the gas, its density and the area of the hole.

        (i) Use dimensional analysis to determine this dependence.

        (ii) If the gas is ideal, how will the rate of loss depend on the molecular weight at a given pressure and temperature?

11. The speed of sound in a gas can be expressed in terms of its pressure and its density.

    (a) Use dimensional analysis to determine this dependence.

    (b) If the gas is ideal, how will the speed of sound depend on the molecular weight at a given temperature?

    (c) The speed of sound in air at room temperature is 330 ms^{-1}. Calculate the speed of sound in gaseous helium at the same temperature.

12. When an oil droplet is released, it falls under the influence of gravity until it reaches its terminal velocity, at which the gravitational force exactly balances the frictional force exerted by the air through which it passes. The terminal velocity depends on the weight mg of the drop (g is the acceleration due to gravity and m is the mass of the droplet), the viscosity η of the medium, and the radius a of the droplet.

    (a) Use dimensional analysis to work out how the terminal velocity should depend on all of these factors.
    [The SI units of viscosity are kg m^{-1} s^{-1}.]

    (b) What will be the effect of the following changes on the terminal velocity?

        (i) Using a gas with twice the viscosity of air.

        (ii) Using an oil drop with double the radius.

13. The rotational energy of a diatomic molecule is a function of its bond length, r, its reduced mass, μ, and Planck's constant, h. Use dimensional analysis to find out how the energy depends on these quantities.

14. The wind chill factor is the reduction in temperature due to the wind speed. It arises from the conversion of random motion (temperature) into organised motion (wind). The wind chill factor ΔT depends on the wind speed, v, the molecular mass of the gas, m, and Boltzmann's constant k, which has the value 1.38×10^{-23} J K^{-1}. Find the dimensions of each of these quantities and use dimensional analysis to discover how ΔT depends on them.

15. The molecular collision frequency per unit concentration in a gas, Z, has units m^3 s^{-1} and depends on the Boltzmann constant, k_B, the temperature, T, the molecular mass, m, and the molecular diameter, d. Use dimensional analysis to determine how Z depends on these quantities.

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Quantities, Units and Symbols in Physical Chemistry

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SECOND EDITION

BLACKWELL SCIENCE

1
Physical quantities and units

1.1 PHYSICAL QUANTITIES AND QUANTITY CALCULUS

The value of a *physical quantity* can be expressed as the product of a *numerical value* and a *unit*:

$$\text{physical quantity} = \text{numerical value} \times \text{unit}$$

Neither the name of the physical quantity, nor the symbol used to denote it, should imply a particular choice of unit.

Physical quantities, numerical values, and units, may all be manipulated by the ordinary rules of algebra. Thus we may write, for example, for the wavelength λ of one of the yellow sodium lines:

$$\lambda = 5.896 \times 10^{-7}\ \mathrm{m} = 589.6\ \mathrm{nm} \tag{1}$$

where m is the symbol for the unit of length called the metre (see chapter 3), nm is the symbol for the nanometre, and the units m and nm are related by

$$\mathrm{nm} = 10^{-9}\ \mathrm{m} \tag{2}$$

The equivalence of the two expressions for λ in equation (1) follows at once when we treat the units by the rules of algebra and recognize the identity of nm and 10^{-9} m in equation (2). The wavelength may equally well be expressed in the form

$$\lambda/\mathrm{m} = 5.896 \times 10^{-7} \tag{3}$$

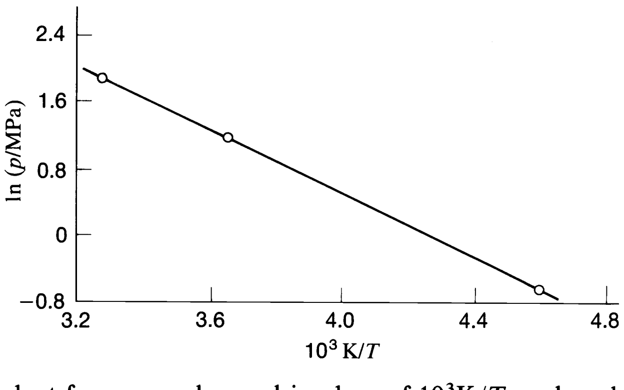
or

$$\lambda/\mathrm{nm} = 589.6 \tag{4}$$

In tabulating the numerical values of physical quantities, or labelling the axes of graphs, it is particularly convenient to use the quotient of a physical quantity and a unit in such a form that the values to be tabulated are pure numbers, as in equations (3) and (4).

Examples

T/K	$10^3\mathrm{K}/T$	p/MPa	$\ln(p/\mathrm{MPa})$
216.55	4.6179	0.5180	−0.6578
273.15	3.6610	3.4853	1.2486
304.19	3.2874	7.3815	1.9990



Algebraically equivalent forms may be used in place of $10^3\mathrm{K}/T$, such as kK/T or $10^3(T/\mathrm{K})^{-1}$.

The method described here for handling physical quantities and their units is known as *quantity calculus*. It is recommended for use throughout science and technology. The use of quantity calculus does not imply any particular choice of units; indeed one of the advantages of quantity calculus is that it makes changes between units particularly easy to follow. Further examples of the use of quantity calculus are given in chapter 7, which is concerned with the problems of transforming from one set of units to another.

1.2 BASE PHYSICAL QUANTITIES AND DERIVED PHYSICAL QUANTITIES

By convention physical quantities are organized in a dimensional system built upon seven *base quantities*, each of which is regarded as having its own dimension. These base quantities and the symbols used to denote them are as follows:

Physical quantity	*Symbol for quantity*
length	l
mass	m
time	t
electric current	I
thermodynamic temperature	T
amount of substance	n
luminous intensity	I_v

All other physical quantities are called *derived quantities* and are regarded as having dimensions derived algebraically from the seven base quantities by multiplication and division.

Example dimension of (energy) = dimension of (mass $\times$ length^2 $\times$ time^{-2})

The physical quantity *amount of substance* or *chemical amount* is of special importance to chemists. Amount of substance is proportional to the number of specified elementary entities of that substance, the proportionality factor being the same for all substances; its reciprocal is the *Avogadro constant* (see sections 2.10, p.46, and 3.2, p.70, and chapter 5). The SI unit of amount of substance is the mole, defined in chapter 3 below. The physical quantity 'amount of substance' should no longer be called 'number of moles', just as the physical quantity 'mass' should not be called 'number of kilograms'. The name 'amount of substance' and 'chemical amount' may often be usefully abbreviated to the single word 'amount', particularly in such phrases as 'amount concentration' (p.42)[1], and 'amount of N_2' (see examples on p.46).

(1) The Clinical Chemistry Division of IUPAC recommends that 'amount-of-substance concentration' be abbreviated 'substance concentration'.

1.3 SYMBOLS FOR PHYSICAL QUANTITIES AND UNITS [5.a]

A clear distinction should be drawn between the names and symbols for physical quantities, and the names and symbols for units. Names and symbols for many physical quantities are given in chapter 2; the symbols given there are *recommendations.* If other symbols are used they should be clearly defined. Names and symbols for units are given in chapter 3; the symbols for units listed there are *mandatory.*

General rules for symbols for physical quantities

The symbol for a physical quantity should generally be a single letter of the Latin or Greek alphabet (see p.143)[1]. Capital and lower case letters may both be used. The letter should be printed in italic (sloping) type. When no italic font is available the distinction may be made by underlining symbols for physical quantities in accord with standard printers' practice. When necessary the symbol may be modified by subscripts and/or superscripts of specified meaning. Subscripts and superscripts that are themselves symbols for physical quantities or numbers should be printed in italic type; other subscripts and superscripts should be printed in roman (upright) type.

Examples		C_p	for heat capacity at constant pressure
		x_i	for mole fraction of the *i*th species
	but	C_B	for heat capacity of substance B
		E_k	for kinetic energy
		μ_r	for relative permeability
		$\Delta_\mathrm{r}H^\circ$	for standard reaction enthalpy
		V_m	for molar volume

The meaning of symbols for physical quantities may be further qualified by the use of one or more subscripts, or by information contained in round brackets.

Examples $\Delta_\mathrm{f}S^\circ(\mathrm{HgCl_2, cr}, 25\,^\circ\mathrm{C}) = -154.3\ \mathrm{J\,K^{-1}\,mol^{-1}}$
$\mu_i = (\partial G/\partial n_i)_{T,p,n_{j\neq i}}$

Vectors and matrices may be printed in bold face italic type, e.g. $\boldsymbol{A}$, $\boldsymbol{a}$. Matrices and tensors are sometimes printed in bold face sans-serif type, e.g. $\boldsymbol{\mathsf{S}}$, $\boldsymbol{\mathsf{T}}$. Vectors may alternatively be characterized by an arrow, $\vec{A}$, $\vec{a}$ and second rank tensors by a double arrow, $\overset{\rightrightarrows}{S}$, $\overset{\rightrightarrows}{T}$.

General rules for symbols for units

Symbols for units should be printed in roman (upright) type. They should remain unaltered in the plural, and should not be followed by a full stop except at the end of a sentence.

Example $r = 10$ cm, not cm. or cms.

Symbols for units should be printed in lower case letters, unless they are derived from a personal name when they should begin with a capital letter. (An exception is the symbol for the litre which may be either L or l, i.e. either capital or lower case.)

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(1) An exception is made for certain dimensionless quantities used in the study of transport processes for which the internationally agreed symbols consist of two letters (see section 2.15).

Example Reynolds number, *Re*

When such symbols appear as factors in a product, they should be separated from other symbols by a space, multiplication sign, or brackets.

Examples m (metre), s (second), but J (joule), Hz (hertz)

Decimal multiples and submultiples of units may be indicated by the use of prefixes as defined in section 3.6 below.

Examples nm (nanometre), kHz (kilohertz), Mg (megagram)

3
Definitions and symbols for units

3.1 THE INTERNATIONAL SYSTEM OF UNITS (SI)

The International System of units (SI) was adopted by the 11th General Conference on Weights and Measures (CGPM) in 1960 [3]. It is a coherent system of units built from seven *SI base units*, one for each of the seven dimensionally independent base quantities (see section 1.2): they are the metre, kilogram, second, ampere, kelvin, mole, and candela, for the dimensions length, mass, time, electric current, thermodynamic temperature, amount of substance, and luminous intensity, respectively. The definitions of the SI base units are given in section 3.2. The *SI derived units* are expressed as products of powers of the base units, analogous to the corresponding relations between physical quantities but with numerical factors equal to unity [3].

In the International System there is only one SI unit for each physical quantity. This is either the appropriate SI base unit itself (see table 3.3) or the appropriate SI derived unit (see tables 3.4 and 3.5). However, any of the approved decimal prefixes, called *SI prefixes*, may be used to construct decimal multiples or submultiples of SI units (see table 3.6).

It is recommended that only SI units be used in science and technology (with SI prefixes where appropriate). Where there are special reasons for making an exception to this rule, it is recommended always to define the units used in terms of SI units.

3.2 DEFINITIONS OF THE SI BASE UNITS [3]

metre: The metre is the length of path travelled by light in vacuum during a time interval of 1/299 792 458 of a second (17th CGPM, 1983).

kilogram: The kilogram is the unit of mass; it is equal to the mass of the international prototype of the kilogram (3rd CGPM, 1901).

second: The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the caesium-133 atom (13th CGPM, 1967).

ampere: The ampere is that constant current which, if maintained in two straight parallel conductors of infinite length, of negligible circular cross-section, and placed 1 metre apart in vacuum, would produce between these conductors a force equal to 2×10^{-7} newton per metre of length (9th CGPM, 1948).

kelvin: The kelvin, unit of thermodynamic temperature, is the fraction 1/273.16 of the thermodynamic temperature of the triple point of water (13th CGPM, 1967).

mole: The mole is the amount of substance of a system which contains as many elementary entities as there are atoms in 0.012 kilogram of carbon-12. When the mole is used, the elementary entities must be specified and may be atoms, molecules, ions, electrons, other particles, or specified groups of such particles (14th CGPM, 1971).

Examples of the use of the mole

1 mol of H_2 contains about 6.022×10^{23} H_2 molecules, or 12.044×10^{23} H atoms
1 mol of HgCl has a mass of 236.04 g
1 mol of Hg_2Cl_2 has a mass of 472.08 g
1 mol of $Hg_2{}^{2+}$ has a mass of 401.18 g and a charge of 192.97 kC
1 mol of $Fe_{0.91}S$ has a mass of 82.88 g
1 mol of e^- has a mass of 548.60 μg and a charge of -96.49 kC
1 mol of photons whose frequency is 5×10^{14} Hz has energy of about 199.5 kJ

See also section 2.10, p.46.

candela: The candela is the luminous intensity, in a given direction, of a source that emits monochromatic radiation of frequency 540×10^{12} hertz and that has a radiant intensity in that direction of (1/683) watt per steradian (16th CGPM, 1979).

3.3 NAMES AND SYMBOLS FOR THE SI BASE UNITS

The symbols listed here are internationally agreed and should not be changed in other languages or scripts. See sections 1.3 and 1.4 on the printing of symbols for units. Recommended representations for these symbols for use in systems with limited character sets can be found in [7].

Physical quantity	*Name of SI unit*	*Symbol for SI unit*
length	metre	m
mass	kilogram	kg
time	second	s
electric current	ampere	A
thermodynamic temperature	kelvin	K
amount of substance	mole	mol
luminous intensity	candela	cd

3.4 SI DERIVED UNITS WITH SPECIAL NAMES AND SYMBOLS

Physical quantity	*Name of SI unit*	*Symbol for SI unit*	*Expression in terms of SI base units*	
frequency[1]	hertz	Hz	s^{-1}	
force	newton	N	$m\,kg\,s^{-2}$	
pressure, stress	pascal	Pa	$N\,m^{-2}$	$= m^{-1}\,kg\,s^{-2}$
energy, work, heat	joule	J	N m	$= m^2\,kg\,s^{-2}$
power, radiant flux	watt	W	$J\,s^{-1}$	$= m^2\,kg\,s^{-3}$
electric charge	coulomb	C	A s	
electric potential, electromotive force	volt	V	$J\,C^{-1}$	$= m^2\,kg\,s^{-3}\,A^{-1}$
electric resistance	ohm	Ω	$V\,A^{-1}$	$= m^2\,kg\,s^{-3}\,A^{-2}$
electric conductance	siemens	S	Ω^{-1}	$= m^{-2}\,kg^{-1}\,s^3\,A^2$
electric capacitance	farad	F	$C\,V^{-1}$	$= m^{-2}\,kg^{-1}\,s^4\,A^2$
magnetic flux density	tesla	T	$V\,s\,m^{-2}$	$= kg\,s^{-2}\,A^{-1}$
magnetic flux	weber	Wb	V s	$= m^2\,kg\,s^{-2}\,A^{-1}$
inductance	henry	H	$V\,A^{-1}\,s$	$= m^2\,kg\,s^{-2}\,A^{-2}$
Celsius temperature[2]	degree Celsius	°C	K	
luminous flux	lumen	lm	cd sr	
illuminance	lux	lx	$cd\,sr\,m^{-2}$	
activity[3] (radioactive)	becquerel	Bq	s^{-1}	
absorbed dose[3] (of radiation)	gray	Gy	$J\,kg^{-1}$	$= m^2\,s^{-2}$
dose equivalent[3] (dose equivalent index)	sievert	Sv	$J\,kg^{-1}$	$= m^2\,s^{-2}$
plane angle[4]	radian	rad	1	$= m\,m^{-1}$
solid angle[4]	steradian	sr	1	$= m^2\,m^{-2}$

(1) For radial (angular) frequency and for angular velocity the unit rad s^{-1}, or simply s^{-1}, should be used, and this may *not* be simplified to Hz. The unit Hz should be used *only* for frequency in the sense of cycles per second.
(2) The Celsius temperature θ is defined by the equation

$$\theta/°C = T/K - 273.15$$

The SI unit of Celsius temperature is the degree Celsius, °C, which is equal to the kelvin, K. °C should be treated as a single symbol, with no space between the ° sign and the letter C. (The symbol °K, and the symbol °, should no longer be used.)
(3) The units becquerel, gray and sievert are admitted for reasons of safeguarding human health [3].
(4) The units radian and steradian are described as 'SI supplementary units' [3]. However, in chemistry, as well as in physics [4], they are usually treated as dimensionless derived units, and this was recognized by CIPM in 1980. Since they are then of dimension 1, this leaves open the possibility of including them or omitting them in expressions of SI derived units. In practice this means that rad and sr may be used when appropriate and may be omitted if clarity is not lost thereby.

3.5 SI DERIVED UNITS FOR OTHER QUANTITIES

This table gives examples of other SI derived units; the list is merely illustrative.

Physical quantity	*Expression in terms of SI base units*	
area	m^2	
volume	m^3	
speed, velocity	$m\,s^{-1}$	
angular velocity	s^{-1}, $rad\,s^{-1}$	
acceleration	$m\,s^{-2}$	
moment of force	$N\,m$	$= m^2\,kg\,s^{-2}$
wavenumber	m^{-1}	
density, mass density	$kg\,m^{-3}$	
specific volume	$m^3\,kg^{-1}$	
amount concentration[1]	$mol\,m^{-3}$	
molar volume	$m^3\,mol^{-1}$	
heat capacity, entropy	$J\,K^{-1}$	$= m^2\,kg\,s^{-2}\,K^{-1}$
molar heat capacity, molar entropy	$J\,K^{-1}\,mol^{-1}$	$= m^2\,kg\,s^{-2}\,K^{-1}\,mol^{-1}$
specific heat capacity, specific entropy	$J\,K^{-1}\,kg^{-1}$	$= m^2\,s^{-2}\,K^{-1}$
molar energy	$J\,mol^{-1}$	$= m^2\,kg\,s^{-2}\,mol^{-1}$
specific energy	$J\,kg^{-1}$	$= m^2\,s^{-2}$
energy density	$J\,m^{-3}$	$= m^{-1}\,kg\,s^{-2}$
surface tension	$N\,m^{-1} = J\,m^{-2}$	$= kg\,s^{-2}$
heat flux density, irradiance	$W\,m^{-2}$	$= kg\,s^{-3}$
thermal conductivity	$W\,m^{-1}\,K^{-1}$	$= m\,kg\,s^{-3}\,K^{-1}$
kinematic viscosity, diffusion coefficient	$m^2\,s^{-1}$	
dynamic viscosity	$N\,s\,m^{-2} = Pa\,s$	$= m^{-1}\,kg\,s^{-1}$
electric charge density	$C\,m^{-3}$	$= m^{-3}\,s\,A$
electric current density	$A\,m^{-2}$	
conductivity	$S\,m^{-1}$	$= m^{-3}\,kg^{-1}\,s^3\,A^2$
molar conductivity	$S\,m^2\,mol^{-1}$	$= kg^{-1}\,mol^{-1}\,s^3\,A^2$
permittivity	$F\,m^{-1}$	$= m^{-3}\,kg^{-1}\,s^4\,A^2$
permeability	$H\,m^{-1}$	$= m\,kg\,s^{-2}\,A^{-2}$
electric field strength	$V\,m^{-1}$	$= m\,kg\,s^{-3}\,A^{-1}$
magnetic field strength	$A\,m^{-1}$	
luminance	$cd\,m^{-2}$	
exposure (X and γ rays)	$C\,kg^{-1}$	$= kg^{-1}\,s\,A$
absorbed dose rate	$Gy\,s^{-1}$	$= m^2\,s^{-3}$

(1) The words 'amount concentration' are an abbreviation for 'amount-of-substance concentration'. When there is not likely to be any ambiguity this quantity may be called simply 'concentration'.

3.6 SI PREFIXES

To signify decimal multiples and submultiples of SI units the following prefixes may be used [3].

Submultiple	*Prefix*	*Symbol*	*Multiple*	*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
10^{-21}	zepto	z	10^{21}	zetta	Z
10^{-24}	yocto	y	10^{24}	yotta	Y

Prefix symbols should be printed in roman (upright) type with no space between the prefix and the unit symbol.

Example kilometre, km

When a prefix is used with a unit symbol, the combination is taken as a new symbol that can be raised to any power without the use of parentheses.

Examples $1\ \mathrm{cm}^3 = (0.01\ \mathrm{m})^3 = 10^{-6}\ \mathrm{m}^3$
$1\ \mu\mathrm{s}^{-1} = (10^{-6}\ \mathrm{s})^{-1} = 10^{6}\ \mathrm{s}^{-1}$
$1\ \mathrm{V/cm} = 100\ \mathrm{V/m}$
$1\ \mathrm{mmol/dm}^3 = 1\ \mathrm{mol\,m}^{-3}$

A prefix should never be used on its own, and prefixes are not to be combined into compound prefixes.

Example pm, not µµm

The names and symbols of decimal multiples and submultiples of the SI base unit of mass, the kg, which already contains a prefix, are constructed by adding the appropriate prefix to the word gram and symbol g.

Examples mg, not µkg; Mg, not kkg

The SI prefixes are not to be used with °C.

ISO has recommended standard representations of the prefix symbols for use with limited character sets [7].

3.7 UNITS IN USE TOGETHER WITH THE SI

These units are not part of the SI, but it is recognized that they will continue to be used in appropriate contexts. SI prefixes may be attached to some of these units, such as millilitre, ml; millibar, mbar; megaelectronvolt, MeV; kilotonne, kt. A more extensive list of non-SI units, with conversion factors to the corresponding SI units, is given in chapter 7.

Physical quantity	*Name of unit*	*Symbol for unit*	*Value in SI units*
time	minute	min	60 s
time	hour	h	3600 s
time	day	d	86 400 s
plane angle	degree	°	$(\pi/180)$ rad
plane angle	minute	′	$(\pi/10\,800)$ rad
plane angle	second	″	$(\pi/648\,000)$ rad
length	ångström[1]	Å	10^{-10} m
area	barn	b	10^{-28} m^2
volume	litre	l, L	dm^3 $=10^{-3}$ m^3
mass	tonne	t	Mg $=10^3$ kg
pressure	bar[1]	bar	10^5 Pa $=10^5$ N m^{-2}
energy	electronvolt[2]	eV $(=e \times \mathrm{V})$	$\approx 1.60218 \times 10^{-19}$ J
mass	unified atomic mass unit[2,3]	u $(=m_a(^{12}\mathrm{C})/12)$	$\approx 1.66054 \times 10^{-27}$ kg

(1) The ångström and the bar are approved by CIPM [3] for 'temporary use with SI units', until CIPM makes a further recommendation. However, they should not be introduced where they are not used at present.
(2) The values of these units in terms of the corresponding SI units are not exact, since they depend on the values of the physical constants e (for the electronvolt) and N_A (for the unified atomic mass unit), which are determined by experiment. See chapter 5.
(3) The unified atomic mass unit is also sometimes called the dalton, with symbol Da, although the name and symbol have not been approved by CGPM.

3.8 ATOMIC UNITS [9] (see also section 7.3, p.120)

For the purposes of quantum mechanical calculations of electronic wavefunctions, it is convenient to regard certain fundamental constants (and combinations of such constants) as though they were units. They are customarily called *atomic units* (abbreviated: au), and they may be regarded as forming a coherent system of units for the calculation of electronic properties in theoretical chemistry, although there is no authority from CGPM for treating them as units. They are discussed further in relation to the electromagnetic units in chapter 7, p.120. The first five atomic units in the table below have special names and symbols. Only four of these are independent; all others may be derived by multiplication and division in the usual way, and the table includes a number of examples.

The relation of atomic units to the corresponding SI units involves the values of the fundamental physical constants, and is therefore not exact. The numerical values in the table are based on the estimates of the fundamental constants given in chapter 5. The numerical results of calculations in theoretical chemistry are frequently quoted in atomic units, or as numerical values in the form (*physical quantity*)/(*atomic unit*), so that the reader may make the conversion using the current best estimates of the physical constants.

Physical quantity	*Name of unit*	*Symbol for unit*	*Value of unit in SI*
mass	electron rest mass	m_e	$9.109\,3897(54) \times 10^{-31}$ kg
charge	elementary charge	e	$1.602\,177\,33(49) \times 10^{-19}$ C
action	Planck constant/2π[1]	$\hbar$	$1.054\,572\,66(63) \times 10^{-34}$ J s
length	bohr[1]	a_0	$5.291\,772\,49(24) \times 10^{-11}$ m
energy	hartree[1]	E_h	$4.359\,7482(26) \times 10^{-18}$ J
time		$\hbar/E_h$	$2.418\,884\,3341(29) \times 10^{-17}$ s
velocity[2]		$a_0E_h/\hbar$	$2.187\,691\,42(10) \times 10^{6}$ m s^{-1}
force		E_h/a_0	$8.238\,7295(25) \times 10^{-8}$ N
momentum, linear		$\hbar/a_0$	$1.992\,8534(12) \times 10^{-24}$ N s
electric current		$eE_h/\hbar$	$6.623\,6211(20) \times 10^{-3}$ A
electric field		E_h/ea_0	$5.142\,2082(15) \times 10^{11}$ V m^{-1}
electric dipole moment		ea_0	$8.478\,3579(26) \times 10^{-30}$ C m
magnetic flux density		$\hbar/ea_0^2$	$2.350\,518\,08(71) \times 10^{5}$ T
magnetic dipole moment[3]		$e\hbar/m_e$	$1.854\,803\,08(62) \times 10^{-23}$ J T^{-1}

(1) $\hbar = h/2\pi$; $a_0 = 4\pi\varepsilon_0\hbar^2/m_ee^2$; $E_h = \hbar^2/m_ea_0^2$.
(2) The numerical value of the speed of light, when expressed in atomic units, is equal to the reciprocal of the fine structure constant α; $c/(\text{au of velocity}) = c\hbar/a_0E_h = \alpha^{-1} \approx 137.035\,9895(61)$.
(3) The atomic unit of magnetic dipole moment is twice the Bohr magneton, μ_B.

3.9 DIMENSIONLESS QUANTITIES

Values of dimensionless physical quantities, more properly called 'quantities of dimension one', are often expressed in terms of mathematically exactly defined values denoted by special symbols or abbreviations, such as % (percent) and ppm (part per million). These symbols are then treated as units, and are used as such in calculations.

Fractions (relative values, yields, efficiencies)

Fractions such as relative uncertainty, mole fraction x (also called amount fraction, or number fraction), mass fraction w, and volume fraction ϕ (see p.41 for all these quantities), are sometimes expressed in terms of the symbols summarized in the table below.

Name	*Symbol*	*Value*	*Examples*
percent	%	10^{-2}	The isotopic abundance of carbon-13 expressed as a mole fraction is $x = 1.1\%$
part per million	ppm	10^{-6}	The relative uncertainty in the Planck constant $h\ (= 6.626\,0755(40) \times 10^{-34}$ J s) is 0.60 ppm
			The mass fraction of impurities in a sample of copper was found to be less than 3 ppm, $w < 3$ ppm

These multiples of the unit one are not part of the SI and ISO recommends that these symbols should never be used. They are also frequently used as units of 'concentration' without a clear indication of the type of fraction implied (e.g. mole fraction, mass fraction or volume fraction). To avoid ambiguity they should only be used in a context where the meaning of the quantity is carefully defined. Even then, the use of an appropriate SI unit ratio may be preferred.

Further examples: (i) The mass fraction $w = 1.5 \times 10^{-6} = 1.5$ ppm, or $w = 1.5$ mg/kg
(ii) The mole fraction $x = 3.7 \times 10^{-2} = 3.7\%$ or $x = 37$ mmol/mol
(iii) Atomic absorption spectroscopy shows the aqueous solution to contain a mass concentration of nickel $\rho(\mathrm{Ni}) = 2.6\ \mathrm{mg\,dm^{-3}}$, which is approximately equivalent to a mass fraction $w(\mathrm{Ni}) = 2.6 \times 10^{-6} = 2.6$ ppm.

Note the importance of using the recommended name and symbol for the quantity in each of the above examples. Statements such as 'the concentration of nickel was 2.6 ppm' are ambiguous and should be avoided.

Example (iii) illustrates the approximate equivalence of (ρ/mg dm^{-3}) and (w/ppm) in aqueous solution, which follows from the fact that the mass density of a dilute aqueous solution is always approximately 1.0 g cm^{-3}. Dilute solutions are often measured or calibrated to a known mass concentration in mg dm^{-3}, and this unit is then to be preferred to using ppm to specify a mass fraction.

Deprecated usage

Adding extra labels to ppm and similar symbols, such as ppmv (meaning ppm by volume) should be avoided. Qualifying labels may be added to symbols for physical quantities, but never to units.

7
Conversion of units

SI units are recommended for use throughout science and technology. However, some non-SI units are in use, and in a few cases they are likely to remain so for many years. Moreover, the published literature of science makes widespread use of non-SI units. It is thus often necessary to convert the values of physical quantities between SI and other units. This chapter is concerned with facilitating this process.

Section 7.1 gives examples illustrating the use of quantity calculus for converting the values of physical quantities between different units. The table in section 7.2 lists a variety of non-SI units used in chemistry, with the conversion factors to the corresponding SI units. Conversion factors for energy and energy-related units (wavenumber, frequency, temperature and molar energy), and for pressure units, are also presented in tables inside the back cover.

Many of the difficulties in converting units between different systems are associated either with the electromagnetic units, or with atomic units and their relationship to the electromagnetic units. In sections 7.3 and 7.4 the relations involving electromagnetic and atomic units are developed in greater detail to provide a background for the conversion factors presented in the table in section 7.2.

7.1 THE USE OF QUANTITY CALCULUS

Quantity calculus is a system of algebra in which symbols are consistently used to represent physical quantities rather, than their measures, i.e. numerical values in certain units. Thus we always take the values of physical quantities to be the product of a numerical value and a unit (see section 1.1), and we manipulate the symbols for physical quantities, numerical values, and units by the ordinary rules of algebra.[1] This system is recommended for general use in science. Quantity calculus has particular advantages in facilitating the problems of converting between different units and different systems of units, as illustrated by the examples below. In all of these examples the numerical values are approximate.

Example 1. The wavelength λ of one of the yellow lines of sodium is given by

$$\lambda = 5.896 \times 10^{-7}\ \mathrm{m}, \quad \text{or} \quad \lambda/\mathrm{m} = 5.896 \times 10^{-7}$$

The ångström is defined by the equation (see table 7.2, under length)

$$1\ \text{Å} = \text{Å} = 10^{-10}\ \mathrm{m}, \quad \text{or} \quad \mathrm{m}/\text{Å} = 10^{10}$$

Substituting in the first equation gives the value of λ in ångström units

$$\lambda/\text{Å} = (\lambda/\mathrm{m})\,(\mathrm{m}/\text{Å}) = (5.896 \times 10^{-7})\,(10^{10}) = 5896$$

or

$$\lambda = 5896\ \text{Å}$$

Example 2. The vapour pressure of water at 20 °C is recorded to be

$$p(\mathrm{H_2O}, 20\ ^\circ\mathrm{C}) = 17.5\ \mathrm{Torr}$$

The torr, the bar, and the atmosphere are given by the equations (see table 7.2, under pressure)

$$\mathrm{Torr} \approx 133.3\ \mathrm{Pa},$$
$$\mathrm{bar} = 10^5\ \mathrm{Pa},$$
$$\mathrm{atm} = 101\,325\ \mathrm{Pa}.$$

Thus

$$\begin{aligned} p(\mathrm{H_2O}, 20\ ^\circ\mathrm{C}) &= 17.5 \times 133.3\ \mathrm{Pa} = 2.33\ \mathrm{kPa} \\ &= (2.33 \times 10^3/10^5)\ \mathrm{bar} = 23.3\ \mathrm{mbar} \\ &= (2.33 \times 10^3/101\,325)\ \mathrm{atm} = 2.30 \times 10^{-2}\ \mathrm{atm} \end{aligned}$$

Example 3. Spectroscopic measurements show that for the methylene radical, $\mathrm{CH_2}$, the $\tilde{a}\ {}^1A_1$ excited state lies at a wavenumber 3156 cm^{-1} above the $\tilde{X}\ {}^3B_1$ ground state

$$\tilde{\nu}(\tilde{a} - \tilde{X}) = T_0(\tilde{a}) - T_0(\tilde{X}) = 3156\ \mathrm{cm}^{-1}$$

The excitation energy from the ground triplet state to the excited singlet state is thus

$$\begin{aligned} \Delta E = hc\tilde{\nu} &= (6.626 \times 10^{-34}\ \mathrm{J\,s})\,(2.998 \times 10^8\ \mathrm{m\,s^{-1}})\,(3156\ \mathrm{cm^{-1}}) \\ &= 6.269 \times 10^{-22}\ \mathrm{J\,m\,cm^{-1}} \\ &= 6.269 \times 10^{-20}\ \mathrm{J} = 6.269 \times 10^{-2}\ \mathrm{aJ} \end{aligned}$$

where the values of h and c are taken from the fundamental physical constants in chapter 5, and we

(1) A more appropriate name for 'quantity calculus' might be 'algebra of quantities', because it is the principles of algebra rather than calculus that are involved.

have used the relation $\mathrm{m} = 100\ \mathrm{cm}$, or $\mathrm{m\ cm^{-1}} = 100$. Since the electronvolt is given by the equation (table 7.2, under energy) $\mathrm{eV} \approx 1.6022 \times 10^{-19}\ \mathrm{J}$, or $\mathrm{aJ} \approx (1/0.16022)\ \mathrm{eV}$

$$\Delta E = (6.269 \times 10^{-2}/0.16022)\ \mathrm{eV} = 0.3913\ \mathrm{eV}$$

Similarly the Hartree energy is given by (table 7.3) $E_\mathrm{h} = \hbar^2/m_\mathrm{e}a_0{}^2 \approx 4.3598\ \mathrm{aJ}$, or $\mathrm{aJ} \approx (1/4.3598)E_\mathrm{h}$, and thus the excitation energy is given in atomic units by

$$\Delta E = (6.269 \times 10^{-2}/4.3598)E_\mathrm{h} = 1.4380 \times 10^{-2}\ E_\mathrm{h}$$

Finally the molar excitation energy is given by

$$\begin{aligned}\Delta E_\mathrm{m} &= L\Delta E \\ &= (6.022 \times 10^{23}\ \mathrm{mol^{-1}})\ (6.269 \times 10^{-2}\ \mathrm{aJ}) \\ &= 37.75\ \mathrm{kJ\ mol^{-1}}\end{aligned}$$

Also, since $\mathrm{kcal} = 4.184\ \mathrm{kJ}$, or $\mathrm{kJ} = (1/4.184)\ \mathrm{kcal}$,

$$\Delta E_\mathrm{m} = (37.75/4.184)\ \mathrm{kcal\ mol^{-1}} = 9.023\ \mathrm{kcal\ mol^{-1}}$$

Note that in this example the conversion factors are not pure numbers, but have dimensions, and involve the fundamental physical constants h, c, e, m_e, a_0 and L. Also in this example the necessary conversion factors could have been taken directly from the table on the inside back cover.

Example 4. The molar conductivity, Λ, of an electrolyte is defined by the equation (see p.60)

$$\Lambda = \kappa/c$$

where κ is the conductivity of the electrolyte solution minus the conductivity of the pure solvent and c is the electrolyte concentration. Conductivities of electrolytes are usually expressed in $\mathrm{S\ cm^{-1}}$ and concentrations in $\mathrm{mol\ dm^{-3}}$; for example, $\kappa(\mathrm{KCl}) = 7.39 \times 10^{-5}\ \mathrm{S\ cm^{-1}}$ for $c(\mathrm{KCl}) = 0.000\,500\ \mathrm{mol\ dm^{-3}}$. The molar conductivity can then be calculated as follows

$$\begin{aligned}\Lambda &= (7.39 \times 10^{-5}\ \mathrm{S\ cm^{-1}})/(0.000\,500\ \mathrm{mol\ dm^{-3}}) \\ &= 0.1478\ \mathrm{S\ mol^{-1}\ cm^{-1}\ dm^3} = 147.8\ \mathrm{S\ mol^{-1}\ cm^2}\end{aligned}$$

since $\mathrm{dm^3} = 1000\ \mathrm{cm^3}$. The above relationship has previously often been, and sometimes still is, written in the form

$$\Lambda = 1000\kappa/c$$

However, in this form the symbols *do not* represent physical quantities, but the *numerical values* of physical quantities in certain units. Specifically, the last equation is true only if Λ is the molar conductivity in $\mathrm{S\ mol^{-1}\ cm^2}$, κ is the conductivity in $\mathrm{S\ cm^{-1}}$, and c is the concentration in $\mathrm{mol\ dm^{-3}}$. This form does not follow the rules of quantity calculus, and should be avoided. The equation $\Lambda = \kappa/c$, in which the symbols represent physical quantities, is true in any units. If it is desired to write the relationship between numerical values it should be written in the form

$$\Lambda/(\mathrm{S\ mol^{-1}\ cm^2}) = \frac{1000\kappa/(\mathrm{S\ cm^{-1}})}{c/(\mathrm{mol\ dm^{-3}})}$$

Example 5. A solution of 0.125 mol of solute B in 953 g of solvent S has a molality m_B given by[2]

$$m_\mathrm{B} = n_\mathrm{B}/m_\mathrm{S} = (0.125/953)\ \mathrm{mol\ g^{-1}} = 0.131\ \mathrm{mol\ kg^{-1}}$$

---

(2) Note the confusion of notation: m_B denotes molality, and m_S denotes mass. However, these symbols are almost always used. See footnote (16) p.42.

The mole fraction of solute is approximately given by

$$x_B = n_B/(n_S + n_B) \approx n_B/n_S = m_B M_S$$

where it is assumed that $n_B \ll n_S$.

If the solvent is water with molar mass 18.015 g mol^{-1}, then

$$x_B \approx (0.131\ \text{mol kg}^{-1})\ (18.015\ \text{g mol}^{-1}) = 2.36\ \text{g/kg} = 0.00236$$

The equations used here are sometimes quoted in the form $m_B = 1000 n_B/m_S$, and $x_B \approx m_B M_S/1000$. However, this is *not* a correct use of quantity calculus because in this form the symbols denote the *numerical values* of the physical quantities in particular units; specifically it is assumed that m_B, m_S and M_S denote numerical values in mol kg^{-1}, g, and g mol^{-1} respectively. A correct way of writing the second equation would, for example, be

$$x_B = (m_B/\text{mol kg}^{-1})\ (M_S/\text{g mol}^{-1})/1000$$

Example 6. For paramagnetic materials the magnetic susceptibility may be measured experimentally and used to give information on the molecular magnetic dipole moment, and hence on the electronic structure of the molecules in the material. The paramagnetic contribution to the molar magnetic susceptibility of a material, χ_m, is related to the molecular magnetic dipole moment m by the Curie relation

$$\chi_m = \chi V_m = \mu_0 N_A m^2/3kT$$

In terms of the irrational susceptibility $\chi^{(ir)}$, which is often used in connection with the older esu, emu, and Gaussian unit systems (see section 7.3 below), this equation becomes

$$\chi_m^{(ir)} = \chi^{(ir)} V_m = (\mu_0/4\pi)\ N_A m^2/3kT$$

Solving for m, and expressing the result in terms of the Bohr magneton μ_B,

$$m/\mu_B = (3k/\mu_0 N_A)^{1/2} \mu_B^{-1} (\chi_m T)^{1/2}$$

Finally, using the values of the fundamental constants μ_B, k, μ_0, and N_A given in chapter 5, we obtain

$$\begin{aligned} m/\mu_B &= 0.7977[\chi_m/(\text{cm}^3\ \text{mol}^{-1})]^{1/2}[T/\text{K}]^{1/2} \\ &= 2.828[\chi_m^{(ir)}/(\text{cm}^3\ \text{mol}^{-1})]^{1/2}\ [T/\text{K}]^{1/2}. \end{aligned}$$

These expressions are convenient for practical calculations. The final result has frequently been expressed in the form

$$m/\mu_B = 2.828\ (\chi_m T)^{1/2}$$

where it is assumed, contrary to the conventions of quantity calculus, that χ_m and T denote the *numerical values* of the molar susceptibility and the temperature in the units cm^3 mol^{-1} and K respectively, and where it is also assumed (but rarely stated) that the susceptibility is defined using the irrational electromagnetic equations (see section 7.3 below).

THE GREEK ALPHABET

Α, α	A, α	*Alpha*	Ν, ν	N, ν	*Nu*
Β, β	B, β	*Beta*	Ξ, ξ	Ξ, ξ	*Xi*
Γ, γ	Γ, γ	*Gamma*	Ο, ο	O, o	*Omicron*
Δ, δ	Δ, δ	*Delta*	Π, π	Π, π	*Pi*
Ε, ε	E, ε	*Epsilon*	Ρ, ρ	P, ρ	*Rho*
Ζ, ζ	Z, ζ	*Zeta*	Σ, σ	Σ, σ	*Sigma*
Η, η	H, η	*Eta*	Τ, τ	T, τ	*Tau*
Θ, ϑ, θ	$\Theta, \vartheta, \theta$	*Theta*	ϒ, υ	Υ, υ	*Upsilon*
Ι, ι	I, ι	*Iota*	Φ, φ, ϕ	Φ, φ, ϕ	*Phi*
Κ, κ	K, κ	*Kappa*	Χ, χ	X, χ	*Chi*
Λ, λ	Λ, λ	*Lambda*	Ψ, ψ	Ψ, ψ	*Psi*
Μ, μ	M, μ	*Mu*	Ω, ω	Ω, ω	*Omega*

PRESSURE CONVERSION FACTORS

	Pa	kPa	bar	atm	Torr	psi
1 Pa =	1	10^{-3}	10^{-5}	$9.869\,23 \times 10^{-6}$	$7.500\,62 \times 10^{-3}$	$1.450\,38 \times 10^{-4}$
1 kPa =	10^3	1	10^{-2}	$9.869\,23 \times 10^{-3}$	7.500 62	0.145 038
1 bar =	10^5	10^2	1	0.986 923	750.062	145.038
1 atm =	101 325	101.325	1.013 25	1	760	14.6959
1 Torr =	133.322	0.133 322	$1.33\,322 \times 10^{-3}$	$1.315\,79 \times 10^{-3}$	1	$1.933\,67 \times 10^{-2}$
1 psi =	6894.76	6.894 76	$6.894\,76 \times 10^{-2}$	$6.804\,60 \times 10^{-2}$	51.715 07	1

Examples of the use of this table:

1 bar = 0.986 923 atm

1 Torr = 133.322 Pa

Note: 1 mmHg = 1 Torr, to better than 2×10^{-7} Torr (see p.112).

ENERGY CONVERSION FACTORS

$E = h\nu = hc\tilde{\nu} = kT$; $E_m = LE$

			wavenumber $\tilde{\nu}$	frequency ν	energy E			molar energy E_m		temperature T
			cm^{-1}	MHz	aJ	eV	E_h	kJ/mol	kcal/mol	K
$\tilde{\nu}$:	1 cm^{-1}	≙	1	$2.997\,925 \times 10^{4}$	$1.986\,447 \times 10^{-5}$	$1.239\,842 \times 10^{-4}$	$4.556\,335 \times 10^{-6}$	$11.962\,66 \times 10^{-3}$	$2.859\,14 \times 10^{-3}$	1.438 769
ν:	1 MHz	≙	$3.335\,64 \times 10^{-5}$	1	$6.626\,076 \times 10^{-10}$	$4.135\,669 \times 10^{-9}$	$1.519\,830 \times 10^{-10}$	$3.990\,313 \times 10^{-7}$	$9.537\,08 \times 10^{-8}$	$4.799\,22 \times 10^{-5}$
	1 aJ	≙	50 341.1	$1.509\,189 \times 10^{9}$	1	6.241 506	0.229 3710	602.2137	143.9325	$7.242\,92 \times 10^{4}$
E:	1 eV	≙	8065.54	$2.417\,988 \times 10^{8}$	0.160 2177	1	$3.674\,931 \times 10^{-2}$	96.4853	23.0605	$1.160\,45 \times 10^{4}$
	1 E_h	≙	219 474.63	$6.579\,684 \times 10^{9}$	4.359 748	27.2114	1	2625.500	627.510	$3.157\,73 \times 10^{5}$
E_m:	1 kJ/mol	≙	83.5935	$2.506\,069 \times 10^{6}$	$1.660\,540 \times 10^{-3}$	$1.036\,427 \times 10^{-2}$	$3.808\,798 \times 10^{-4}$	1	0.239 006	120.272
	1 kcal/mol	≙	349.755	$1.048\,539 \times 10^{7}$	$6.947\,700 \times 10^{-3}$	$4.336\,411 \times 10^{-2}$	$1.593\,601 \times 10^{-3}$	4.184	1	503.217
T:	1 K	≙	0.695 039	$2.083\,67 \times 10^{4}$	$1.380\,658 \times 10^{-5}$	$8.617\,38 \times 10^{-5}$	$3.166\,83 \times 10^{-6}$	$8.314\,51 \times 10^{-3}$	$1.987\,22 \times 10^{-3}$	1

Examples of the use of this table: 1 aJ ≙ 50 341 cm^{-1}
1 eV ≙ 96.4853 kJ mol^{-1}

The symbol ≙ should be read as meaning 'corresponds to' or 'is equivalent to'