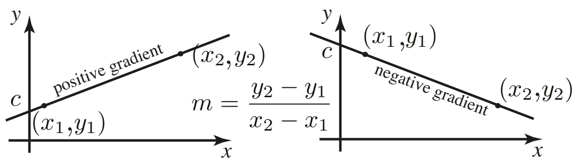
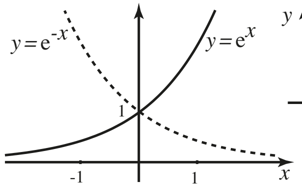
Graphs of common functions

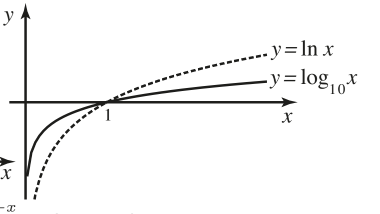
The straight line: $y = mx + c$.
m=gradient (slope), $c =$ vertical intercept.



Exponential and log functions:
e ≈ 2.718 is the exponential constant.

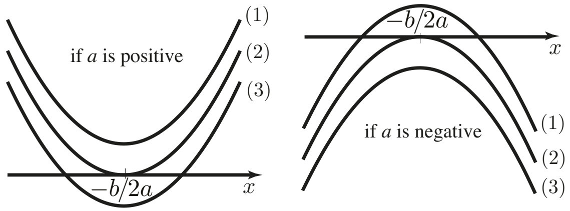


Graph of $y = e^x$ and $y = e^{-x}$
showing exponential growth/ decay



Graph of $y = \ln x$ and $y = \log_{10} x$

Quadratic functions: $y = ax^2 + bx + c$



(1)	$b^2 - 4ac < 0$	(1)	$b^2 - 4ac > 0$
(2)	$b^2 - 4ac = 0$	(2)	$b^2 - 4ac = 0$
(3)	$b^2 - 4ac > 0$	(3)	$b^2 - 4ac < 0$

Statistics

Population values, or **parameters**, are denoted by Greek letters. Population mean $= \mu$. Population variance $= \sigma^2$. Population standard deviation $= \sigma$. Sample values, or **estimates**, are denoted by roman letters.
The **mean** of a sample of n observations $x_1, x_2, \ldots x_n$ is

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} = \frac{x_1 + x_2 + \cdots + x_n}{n}$$

The sample mean $\bar{x}$ is an unbiased estimate of the population mean μ. The unbiased estimate of the **variance** of these n sample observations is $s^2 = \dfrac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1}$ which can be written as

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n} x_i^2 - \frac{n\bar{x}^2}{n-1}$$

The sample unbiased estimate of **standard deviation**, s, is the square root of the variance: $s = \sqrt{\dfrac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n-1}}$. The standard deviation of the sample mean is called the **standard error of the mean** and is equal to $\frac{\sigma}{\sqrt{n}}$, and is often estimated by $\frac{s}{\sqrt{n}}$.

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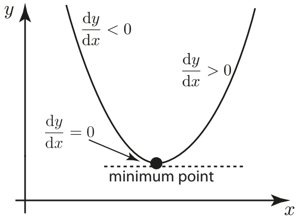
Differentiation

Differentiating a function, $y = f(x)$, we obtain its derivative $\frac{dy}{dx}$. This new function tells us the gradient (slope) of the original function at any point. When $\frac{dy}{dx} = 0$ the gradient is zero.

$y = f(x)$	$\frac{dy}{dx} = f'(x)$
k, constant	0
x	1
x^2	$2x$
x^n, constant n	nx^{n-1}
$\sin(kx)$	$k\cos(kx)$
$\cos(kx)$	$-k\sin(kx)$
e^x	e^x
e^{kx}	ke^{kx}
$\ln kx = \log_e kx$	$\frac{1}{x}$



The linearity rules:

$$\frac{d}{dx}(u(x) \pm v(x)) = \frac{du}{dx} \pm \frac{dv}{dx} \qquad \frac{d}{dx}(k \times f(x)) = k \times \frac{df}{dx}$$

for k constant.

The product and quotient rules:

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx} \qquad \frac{d}{dx}\left(\frac{u}{v}\right) = \frac{v\frac{du}{dx} - u\frac{dv}{dx}}{v^2}.$$

The chain rule:
If $y = y(u)$ where $u = u(x)$ then $\frac{dy}{dx} = \frac{dy}{du} \times \frac{du}{dx}$.

Higher derivatives: $f''(x)$, or $\dfrac{d^2 f}{dx^2}$, means differentiate $\dfrac{df}{dx}$ with respect to x. That is, $\dfrac{d^2 f}{dx^2} = \dfrac{d}{dx}\left(\dfrac{df}{dx}\right)$.

Partial derivatives: If $f = f(x, y)$ is a function of two (or more) independent variables, $\frac{\partial f}{\partial x}$ means differentiate f with respect to x treating y as if it were a constant. $\frac{\partial f}{\partial y}$ means differentiate f with respect to y treating x as if it were a constant.

Integration

$f(x)$	$\int f(x)\,dx$
k, constant	$kx + c$
x	$\frac{x^2}{2} + c$
x^2	$\frac{x^3}{3} + c$
x^n, $(n \neq -1)$	$\frac{x^{n+1}}{n+1} + c$
$x^{-1} = \frac{1}{x}$	$\ln x + c$ or $\ln c'x$
e^x	$e^x + c$
e^{kx}	$\frac{e^{kx}}{k} + c$
$\sin kx$	$-\frac{1}{k}\cos kx + c$
$\cos kx$	$\frac{1}{k}\sin kx + c$

The linearity rule:

$$\int (af(x) + bg(x))\,dx = a\int f(x)\,dx + b\int g(x)\,dx, \qquad (a, b\,\text{constant})$$

Integration by parts: $\displaystyle\int_a^b u\frac{dv}{dx}dx = [uv]_a^b - \int_a^b \frac{du}{dx}v\,dx.$

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Mixtures

Raoult's law: states that the partial vapour pressure, p_A, in a liquid mixture, A, is proportional to its mole fraction, x_A, and its vapour pressure when pure, p_A^*: $p_A = x_A p_A^*$.

Henry's law: states that the vapour pressure, p_B, of a volatile solute, B, is proportional to its mole fraction, x_B, in a solution: $p_B = x_B K_B$. Here K_B is Henry's law constant.

Chemical potential of a solvent:

$$\mu_A = \mu_A^* + RT\,\ln x_A$$

where μ_A^* = chemical potential of pure A and x_A is the mole fraction.

Properties of mixtures: suppose an amount n_A of substance A is mixed with n_B of substance B. The total volume of the mixture is

$$V = n_A\,V_{m,A} + n_B\,V_{m,B}$$

where $V_{m,A}$ = partial molar volume of A and $V_{m,B}$ = partial molar volume of B. More generally, $V = \sum_i n_i V_{m,i}$, where $V_{m,i}$ is the partial molar volume of the ith substance.

Total Gibbs energy for the mixture is $G = n_A\,G_A + n_B\,G_B$ where G_A and G_B are the **partial molar Gibbs energies** of substances A and B respectively. The partial molar Gibbs energies are also denoted μ_A and μ_B so that $G = n_A\,\mu_A + n_B\,\mu_B$. More generally, with mixtures of several substances $G = \sum_i n_i \mu_i$.

Reaction Thermodynamics

Standard state: The standard state of a substance is the pure substance at a pressure of 1 bar. The standard state value is denoted by the superscript symbol $\ominus$, as in $G^{\ominus}$.

Reaction Gibbs energy: $\Delta_r G = \dfrac{\Delta G}{\Delta \xi}$ is the slope of the graph of Gibbs energy against the progress of the reaction. Here, $\Delta\xi = \Delta n_{\mathrm{J}}/\nu_{\mathrm{J}}$ for all species J in the reaction. Reaction Gibbs energy at any composition of the reaction mixture can be written

$$\Delta_r G = \Delta_r G^{\ominus} + RT\ln Q \qquad \text{where } Q = \prod_{\mathrm{J}} a_{\mathrm{J}}^{\nu_{\mathrm{J}}}$$

where a_{J} is the activity of species J and ν_{J} is its stoichiometric number.

At equilibrium $Q = K$, $\Delta_r G = 0$ and $-\Delta_r G^{\ominus} = RT\ln K$ where

$$K = \prod_{\mathrm{J}} (a_{\mathrm{J}}^{v_{\mathrm{J}}})_{\text{equilibrium}}$$

van't Hoff equation: $\dfrac{\mathrm{d}}{\mathrm{d}T}\ln K = \dfrac{\Delta_r H^{\ominus}}{RT^2}$.

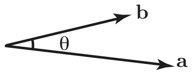
$$\ln\left(\frac{K_2}{K_1}\right) = -\frac{\Delta_r H^{\ominus}}{R}\left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$

Vectors

If $\mathbf{r} = x\mathbf{i} + y\mathbf{j} + z\mathbf{k}$ then $|\mathbf{r}| = \sqrt{x^2+y^2+z^2}$.

Scalar product:

$\mathbf{a}\cdot\mathbf{b} = |\mathbf{a}|\,|\mathbf{b}|\cos\theta$

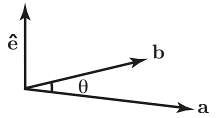


If $\mathbf{a} = a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$ and $\mathbf{b} = b_1\mathbf{i} + b_2\mathbf{j} + b_3\mathbf{k}$ then

$$\mathbf{a}\cdot\mathbf{b} = a_1b_1 + a_2b_2 + a_3b_3$$

Vector product:

$\mathbf{a}\times\mathbf{b} = |\mathbf{a}|\,|\mathbf{b}|\sin\theta\,\hat{\mathbf{e}}$



$\hat{\mathbf{e}}$ is a unit vector perpendicular to the plane containing $\mathbf{a}$ and $\mathbf{b}$ in a sense defined by the right hand screw rule.
If $\mathbf{a} = a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$ and $\mathbf{b} = b_1\mathbf{i} + b_2\mathbf{j} + b_3\mathbf{k}$ then

$$\begin{aligned}\mathbf{a}\times\mathbf{b} &= (a_2b_3 - a_3b_2)\mathbf{i} + (a_3b_1 - a_1b_3)\mathbf{j} + (a_1b_2 - a_2b_1)\mathbf{k} \\ &= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix}\end{aligned}$$

Kinetics

Arrhenius equation: The **rate** at which most chemical reactions proceed depends upon the **temperature**. The amount of energy necessary for the reaction to take place at all is called the **activation energy**. These quantities are related by the Arrhenius equation: $k = A\mathrm{e}^{-E_a/(RT)}$

where k = rate constant, E_a = the activation energy for the reaction, R = ideal gas constant, T = absolute temperature, and A is a constant.

By taking logarithms this can be expressed as

$$\ln\frac{k}{k^{\ominus}} = \ln\frac{A}{k^{\ominus}} - \frac{E_a}{RT}$$

where $k^{\ominus}$ is a chosen standard rate constant. Together, A and E_a are called the **Arrhenius parameters**.

Rate Laws

In the table, $[A]$ = molar concentration of reactant A at time t. $[A]_0$ = concentration of reactant A at time $t = 0$.

Order	Rate Law Differential form	Rate Law Integrated form	Half-life	Common unit of k
0	$\frac{\mathrm{d}[A]}{\mathrm{d}t} = -k$	$[A]_0 - [A] = kt$	$\frac{[A]_0}{2k}$	mol dm^{-3} s^{-1}
1	$\frac{\mathrm{d}[A]}{\mathrm{d}t} = -k[A]$	$[A] = [A]_0\mathrm{e}^{-kt}$	$\frac{\ln 2}{k}$	s^{-1}
2	$\frac{\mathrm{d}[A]}{\mathrm{d}t} = -k[A]^2$	$\frac{1}{[A]} - \frac{1}{[A]_0} = kt$	$\frac{1}{k[A]_0}$	mol^{-1} dm^{3} s^{-1}
2*	$\frac{\mathrm{d}[A]}{\mathrm{d}t} = -k[A][B]$	$\frac{1}{[B]_0-[A]_0}\ln\frac{[B][A]_0}{[A][B]_0} = kt$	-	mol^{-1} dm^{3} s^{-1}

(* $A + B \rightarrow P$ reaction.)

The Greek alphabet

A	α	alpha	I	ι	iota	P	ρ	rho
B	β	beta	K	κ	kappa	Σ	σ	sigma
Γ	γ	gamma	Λ	λ	lambda	T	τ	tau
Δ	δ	delta	M	μ	mu	Υ	υ	upsilon
E	ϵ	epsilon	N	ν	nu	Φ	ϕ	phi
Z	ζ	zeta	Ξ	ξ	xi	X	χ	chi
H	η	eta	O	o	omicron	Ψ	ψ	psi
Θ	θ	theta	Π	π	pi	Ω	ω	omega

Physical constants

Avogadro constant	$N_{\mathrm{A}} = 6.022\times10^{23}$ mol^{-1}
Boltzmann constant	$k_{\mathrm{B}} = 1.381\times10^{-23}$ J K^{-1}
Planck constant	$h = 6.626\times10^{-34}$ J s
Elementary charge	$e = 1.602\times10^{-19}$ C
Ideal gas constant	$R = 8.314$ J K^{-1}mol^{-1}
Vacuum permittivity	$\epsilon_0 = 8.854\times10^{-12}$ J^{-1} C^2 m^{-1}
Speed of light (vacuum)	$c = 2.998\times10^{8}$ m s^{-1}
Faraday constant	$F = e\,N_{\mathrm{A}} = 96.485$ kC mol^{-1}

General Thermodynamics

First Law: For a closed system, $\Delta U = q + w$. Here ΔU is the change in internal energy of a system, w is the work done on the system, and q is the heat energy transferred to the system.

Enthalpy: $H = U + pV$ where U = internal energy, p=pressure and V = volume.

Heat capacity at constant volume: $C_V = \left(\frac{\partial U}{\partial T}\right)_V$

Heat capacity at constant pressure: $C_p = \left(\frac{\partial H}{\partial T}\right)_p$

In general C_p depends upon T. Values of C_p at temperatures not much different from room temperature can be estimated from

$$C_p = a + bT + \frac{c}{T^2}$$

where a, b and c are experimentally determined constants.

Second Law of thermodynamics:

During a spontaneous change, the total entropy of an isolated system and its surroundings increases: $\Delta S > 0$. For a reversible process, at constant temperature, T, change in entropy

$$\Delta S = \frac{q_{rev}}{T}$$

where q_{rev} = energy reversibly transferred as heat.

Boltzmann formula: $S = k_B\ln W$ where W = 'weight' of the most probable configuration of the system and k_B is the Boltzmann constant.

Helmholtz energy: $A = U - TS$.

Gibbs energy: $G = H - TS$.

Change in Gibbs energy: $\Delta G = \Delta H - T\Delta S$ (at constant temperature).

Entropy change for isothermal expansion of an ideal gas:

$$\Delta S = nR\ln\left(\frac{V_{\text{final}}}{V_{\text{initial}}}\right)$$

where V_{final} and V_{initial} are the final and initial volumes.

Gibbs-Helmholtz equation: $\left(\dfrac{\partial}{\partial T}\left(\dfrac{\Delta G}{T}\right)\right)_p = -\dfrac{\Delta H}{T^2}$.

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Arithmetic

When multiplying or dividing positive and negative numbers the sign of the result is given by:

$\text{positive} \times \text{positive} = \text{positive}$ $\quad$ $\text{positive} \times \text{negative} = \text{negative}$
$\text{negative} \times \text{positive} = \text{negative}$ $\quad$ $\text{negative} \times \text{negative} = \text{positive}$

$$\frac{\text{positive}}{\text{positive}} = \text{positive} \qquad \frac{\text{positive}}{\text{negative}} = \text{negative}$$

$$\frac{\text{negative}}{\text{positive}} = \text{negative} \qquad \frac{\text{negative}}{\text{negative}} = \text{positive}$$

The BODMAS rule reminds us of the order in which operations are carried out. BODMAS stands for:

Brackets ()	First priority
Of	Second priority
Division ÷	Second priority
Multiplication ×	Second priority
Addition +	Third priority
Subtraction −	Third priority

Fractions:

$$\text{fraction} = \frac{\text{numerator}}{\text{denominator}}$$

Adding and subtracting fractions: to add or subtract two fractions first rewrite each fraction so that they have the same denominator. Then, the numerators are added or subtracted as appropriate and the result is divided by the common denominator: e.g. $\frac{4}{5} + \frac{3}{4} = \frac{16}{20} + \frac{15}{20} = \frac{31}{20}$.

Multiplying fractions: to multiply two fractions, multiply their numerators and then multiply their denominators: e.g.

$$\frac{3}{7} \times \frac{5}{11} = \frac{3 \times 5}{7 \times 11} = \frac{15}{77}$$

Dividing fractions: to divide two fractions, invert the second and then multiply: e.g. $\frac{3}{5} \div \frac{2}{3} = \frac{3}{5} \times \frac{3}{2} = \frac{9}{10}$.

Proportion and Percentage:

To convert a fraction to a percentage multiply by 100 and label the result as a percentage.

$\frac{5}{8}$ as a percentage is $\frac{5}{8} \times 100\% = 62.5\%$
$\frac{1}{3}$ as a percentage is $\frac{1}{3} \times 100\% = 33\frac{1}{3}\%$

Some common conversions are:

$$\frac{1}{10} = 10\%, \quad \frac{1}{4} = 25\%, \quad \frac{1}{2} = 50\%, \quad \frac{3}{4} = 75\%$$

Ratios are an alternative way of expressing fractions. Consider dividing £200 between two people in the ratio of 3:2. For every £3 the first person gets, the second person gets £2. So the first gets $\frac{3}{5}$ of the total, and the second gets $\frac{2}{5}$ of the total; that is £120 and £80.

Generally, to split a quantity in the ratio $m : n$, the quantity is split into $\frac{m}{m+n}$ of the total and $\frac{n}{m+n}$ of the total.

Trigonometry

Degrees and radians:

$$360^\circ = 2\pi \text{ radians}, \quad 1^\circ = \frac{2\pi}{360} = \frac{\pi}{180} \text{ radians}$$

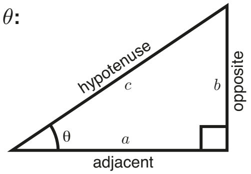
$$1 \text{ radian} = \frac{180}{\pi} \text{ degrees} \approx 57.3^\circ$$

Trig ratios for an acute angle θ:

$$\sin\theta = \frac{\text{side opposite to } \theta}{\text{hypotenuse}} = \frac{b}{c}$$

$$\cos\theta = \frac{\text{side adjacent to } \theta}{\text{hypotenuse}} = \frac{a}{c}$$

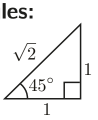
$$\tan\theta = \frac{\text{side opposite to } \theta}{\text{side adjacent to } \theta} = \frac{b}{a}$$

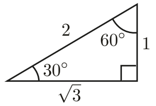


Pythagoras' theorem:

$$a^2 + b^2 = c^2$$

Standard triangles:





$$\sin 45^\circ = \frac{1}{\sqrt{2}}, \qquad \cos 45^\circ = \frac{1}{\sqrt{2}}, \qquad \tan 45^\circ = 1$$

$$\sin 30^\circ = \frac{1}{2}, \qquad \cos 30^\circ = \frac{\sqrt{3}}{2}, \qquad \tan 30^\circ = \frac{1}{\sqrt{3}}$$

$$\sin 60^\circ = \frac{\sqrt{3}}{2}, \qquad \cos 60^\circ = \frac{1}{2}, \qquad \tan 60^\circ = \sqrt{3}$$

Bragg's Law: a fundamental law of x-ray crystallography.

$$n\lambda = 2d\sin\theta$$

λ = wavelength of the x-rays incident on a crystal lattice with planes a distance d apart, n is an integer (whole number), and θ, the Bragg angle, is the angle between the incident beam and the reflecting planes.

Matrices and Determinants

The 2×2 matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ has determinant

$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

The 3×3 matrix $A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$ has determinant

$$|A| = a_{11}\begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12}\begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13}\begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

The inverse of a 2×2 matrix:

If $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ then $A^{-1} = \frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

provided that $ad - bc \neq 0$.

Matrix multiplication: for 2×2 matrices

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} = \begin{pmatrix} a\alpha + b\beta & a\gamma + b\delta \\ c\alpha + d\beta & c\gamma + d\delta \end{pmatrix}$$

Remember that $AB \neq BA$ except in special cases.

Algebra

Removing brackets:

$$a(b + c) = ab + ac, \qquad a(b - c) = ab - ac$$

$$(a + b)(c + d) = ac + ad + bc + bd \qquad \left(\frac{a}{b}\right)c = \frac{ac}{b}$$

Formula for solving a quadratic equation:

$$\text{if } ax^2 + bx + c = 0 \text{ then } x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Laws of Indices:

$$a^m a^n = a^{m+n} \quad \frac{a^m}{a^n} = a^{m-n} \quad (a^m)^n = a^{mn} \quad (ab)^n = a^n b^n$$

$$a^0 = 1 \qquad a^{-m} = \frac{1}{a^m} \qquad a^{1/n} = \sqrt[n]{a} \qquad a^{\frac{m}{n}} = (\sqrt[n]{a})^m$$

Logarithms: for any positive base b (with $b \neq 1$)

$$\log_b A = c \quad \text{means} \quad A = b^c.$$

Logarithms to base e, denoted $\log_e$ or alternatively $\ln$ are called *natural logarithms*. The letter e stands for the exponential constant which is approximately 2.718.

$$\log_e A \text{ or } \ln A = c \text{ means } A = e^c.$$

c, the natural logarithm of a number A, is the power to which e would have to be raised to equal A. Note:

$$e^{\ln A} = A \quad \text{if} \quad A > 0; \qquad \ln(e^A) = A$$

Logarithms to base 10: $\log_{10} A = c$ means $A = 10^c$.

pH: of a solution measures its acidity or basicity.

$$\text{pH} = -\log_{10}([\text{H}^+]/c^\ominus) \quad \text{so} \quad [\text{H}^+] = 10^{-\text{pH}}c^\ominus$$

where $[\text{H}^+]$ = hydrogen ion concentration in mol dm^{-3} and $c^\ominus = 1$ mol dm^{-3}. Equivalently, $\text{pH} = -\log_{10} a_{\text{H}_3\text{O}^+}$ where $a_{\text{H}_3\text{O}^+}$ = hydronium ion activity.

Laws of Logarithms: for any positive base b, with $b \neq 1$,

$$\log_b A + \log_b B = \log_b AB, \qquad \log_b A - \log_b B = \log_b \frac{A}{B},$$

$$n \log_b A = \log_b A^n, \qquad \log_b 1 = 0, \qquad \log_b b = 1.$$

Formula for change of base: $\log_a x = \frac{\log_b x}{\log_b a}$. Specifically, $\log_{10} x = \frac{\ln x}{\ln 10}$.

Inequalities: $a > b$ means a is greater than b
$a < b$ means a is less than b
$a \geqslant b$ means a is greater than or equal to b
$a \leqslant b$ means a is less than or equal to b

Sigma notation: The Greek letter sigma, Σ, is used to abbreviate addition. If we have n values, $x_1, x_2, \ldots x_n$, and add them, the sum $x_1 + x_2 + \ldots x_n$ is written $\sum_{i=1}^{n} x_i$.

Note that i takes all whole number values from 1 to n. So, for instance $\sum_{i=1}^{3} x_i$ means $x_1 + x_2 + x_3$.

Example: $\sum_{i=1}^{5} i^2$ means $1^2 + 2^2 + 3^2 + 4^2 + 5^2$.

Product notation: $\prod_{i=1}^{n} x_i = x_1 \cdot x_2 \cdot \ldots \cdot x_n$.

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Units & Conversions

Scientific notation: is used to express large or small numbers concisely. Each number is written in the form $a \times 10^n$ where a is usually a number between 1 and 10. We make use of

$$\ldots 0.01 = 10^{-2}, 0.1 = 10^{-1}, \ldots, 100 = 10^2, 1000 = 10^3, \ldots$$

Then, for example, $6859 = 6.859 \times 1000 = 6.859 \times 10^3$ and $0.0932 = 9.32 \times 0.01 = 9.32 \times 10^{-2}$.

SI base units: for most quantities it is necessary to specify the **units** in which they are measured.

Quantity	SI unit	Symbol
length	metre	m
mass	kilogram	kg
time	second	s
temperature	kelvin	K
amount of substance	mole	mol
current	ampere	A
luminous intensity	candela	cd

Derived units are formed from the base units. For example, the unit of force is found by combining units of mass, length and time in the combination $\mathrm{kg\,m\,s^{-2}}$. This combination is more usually known as the newton, N.

Property	unit name	unit symbols
frequency	hertz	$\mathrm{Hz = s^{-1}}$
force	newton	$\mathrm{N = kg\,m\,s^{-2}}$
pressure	pascal	$\mathrm{Pa = N\,m^{-2}}$
energy	joule	$\mathrm{J = N\,m = kg\,m^2\,s^{-2}}$
charge	coulomb	A s
potential difference	volt	$\mathrm{V = J\,C^{-1}}$
power	watt	$\mathrm{W = J\,s^{-1}}$
Celsius temperature	degree Celsius	°C
Capacitance	farad	$\mathrm{F = C\,V^{-1}}$
Resistance	ohm	Ω

Common prefixes: a prefix is a method of multiplying the SI unit by an appropriate power of 10 to make it larger or smaller.

Multiple	Prefix	Symbol	Multiple	Prefix	Symbol
10^{12}	tera	T	10^{-1}	deci	d
10^9	giga	G	10^{-2}	centi	c
10^6	mega	M	10^{-3}	milli	m
10^3	kilo	k	10^{-6}	micro	μ
10^2	hecto	h	10^{-9}	nano	n
10^1	deca	da	10^{-12}	pico	p

Interconversion of units:

Sometimes alternative sets of units are used and conversion between these is needed.

Pressure is often quoted in units corresponding to the Standard atmosphere (atm).

Then 1 atm $= 1.01325 \times 10^5$ Pa $= 1.01325$ bar $= 760$mm Hg $=$ 760 Torr. (1 bar $= 1 \times 10^5$ Pa).

Length (of bonds) is sometimes quoted in Ångströms, Å where $1\ \text{Å} = 10^{-10}$ m. 1 nm $= 10^{-9}$m. 0.1nm=100pm.

Energy is often measured in calories (cal): 1 cal $= 4.184$ J.

Amount of substance etc.

The **mole** is the **amount of substance** that contains 6.0221415×10^{23} (Avogadro constant/ $\mathrm{mol^{-1}}$) atoms or molecules of the pure substance being measured. For example 1 mole (mol) of potassium will contain N_A atoms. 1 mole of water contains N_A water molecules. A mole of any substance contains as many atoms or molecules (as specified) as there are atoms in 12g of the carbon isotope $^{12}_{6}$C. (To avoid confusion, always specify the type of particle.)

The **molar mass**, M, of a substance is the mass divided by chemical amount. For pure materials, molar mass, M = molecular weight (or relative atomic or molecular mass) $\times$ $\mathrm{g\,mol^{-1}}$.

The **concentration** or **molarity** of a solute is $c = \frac{n}{V}$ where n = amount of solute, V = volume of <u>solution</u>. Molarity is usually quoted in $\mathrm{mol\,dm^{-3}}$. The unit 1 $\mathrm{mol\,dm^{-3}}$ is commonly denoted 1 M and read as 'molar'.

The **molality**, b, of a solute is the amount of solute divided by the mass of <u>solvent</u>: $b = \frac{n}{m}$. So, molality represents 1 mole of a solute in 1 kg of solvent.

The **mole fraction**, x, of a solute is the amount of solute divided by the total amount in the solution:

$$x = \frac{n}{n_\text{total}}.$$

The **mass density** (or just **density**), ρ, of a substance is its mass divided by its volume, that is $\rho = \frac{m}{V}$.

The **mass percentage** is the mass of a substance in a mixture as a percentage of the total mass of the mixture.

The **mass-volume percentage** is the number of grams of solute in 100 millilitres of solution.

The **volume-volume percentage** is the number of millilitres of liquid solute in 100 millilitres of solution.

Parts per million (ppm): mg/kg.

Parts per billion (ppb): μg/kg.

Yield:
$$\%\ \text{yield} = \frac{\text{Mass obtained}}{\text{Theoretical yield}} \times 100$$

Gases

The general form of an **equation of state** is $p = f(T, V, n)$ where p = pressure, T is temperature, V = volume, n = amount of substance.

Boyle's Law relates the pressure and volume of a gas when the temperature is fixed: $p_1V_1 = p_2V_2$.

An equivalent form is: $pV = \frac{1}{3}nM\overline{c^2}$, where n = number of molecules, m = mass of a molecule, M $(= mN_A)$ is the molar mass of the molecules, $\overline{c^2}$ = mean square speed.

Charles's Law relates the volume and temperature of a gas at constant pressure: $\frac{V_1}{V_2} = \frac{T_1}{T_2}$.

Dalton's Law of partial pressures: states that the pressure exerted by a mix of ideal gases is the sum of the partial pressures each would exert if they were alone in the same volume:

$$p_\text{total} = p_1 + p_2 + \ldots + p_n \qquad \text{or} \qquad p_\text{total} = \sum_{i=1}^{n} p_i$$

The partial pressure, p_i, of one of the gases can be calculated by multiplying the gas mole fraction, x_i, by the total pressure of all the gases, p_total.

Perfect Gas Law: $pV = nRT$ where R = ideal gas constant.

Combined Gas Laws: $\frac{p_1V_1}{T_1} = \frac{p_2V_2}{T_2}$.

Virial equation of state: This improves the perfect gas law because it takes into account intermolecular forces.

$$pV_m = RT(1 + \frac{B}{V_m} + \frac{C}{V_m^2} + \ldots)$$

$V_m = \frac{V}{n}$ = molar volume, B, C etc are the **virial coefficients**. Observe that when the molar volume is very large, the terms $\frac{B}{V_m}$ and $\frac{C}{V_m^2}$ become increasingly less important, and in the limit we obtain the ideal gas law.

Van der Waals equation takes into account the finite distance between molecules and interparticle attractions:

$$p = \frac{RT}{V_m - b} - \frac{a}{V_m^2} \quad \text{or} \quad \left(p + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

a is a measure of attraction between particles, b is the volume excluded by a mole of particles.

Phases

Gibbs' phase rule: $F = C - P + 2$, where F is the number of degrees of freedom, C = number of independent components, P = the number of phases in equilibrium with each other. This is a relationship used to determine the number of state variables, F, chosen from amongst temperature, pressure and species compositions in each phase, which must be specified to fix the thermodynamic state of a system in equilibrium.

Clapeyron equation relates change in pressure to change in temperature at a phase boundary. The slope of the phase boundary is $\frac{\mathrm{d}p}{\mathrm{d}T}$.

$$\frac{\mathrm{d}p}{\mathrm{d}T} = \frac{\Delta H}{T\Delta V}$$

Here ΔH = molar enthalpy of transition, ΔV = change in molar volume during transition.

Clausius-Clapeyron equation is an approximation of the Clapeyron equation for a liquid-vapour phase boundary. Plotting vapour pressure for various temperatures produces a curve. For pure liquids, plotting $\ln \frac{p}{p^\ominus}$ against $\frac{1}{T}$ produces a straight line with gradient $-\frac{\Delta H}{R}$. (Here, $p^\ominus$ = any standard pressure).

$$\ln \frac{p_1}{p_2} = -\frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

Here ΔH = molar enthalpy of vaporisation. This equation relates the natural logarithm of the vapour pressure to the temperature at a phase boundary.