

Energy is often measured in calories (cal): 1 cal = 4.184 J. 1 Å = 10^{−10} m. 1 nm = 10^{−9}m. 0.1nm=100pm. **Length** (of bonds) is sometimes quoted in Ångströms, Å where 760 Torr. (1 bar = 1 × 10⁵ Pa). Then 1 atm = 1.01325 × 10⁵ Pa = 1.01325 bar = 760mm Hg = Standard atmosphere (atm). **Pressure** is often quoted in units corresponding to the between these is needed.

Sometimes alternative sets of units are used and conversion **Interconversion of units:**

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

unit by an appropriate power of 10 to make it larger or smaller. **Common prefixes:** a prefix is a method of multiplying the SI unit by an appropriate power of 10 to make it larger or smaller. Resistance ohm Ω Capacitance farad F = C V^{−1} Celsius temperature degree Celsius °C power watt W = J s^{−1} potential difference volt V = J C^{−1} charge coulomb As energy joule J = N m = kg m² s^{−2} pressure pascal Pa = N m^{−2} force newton N = kg m s^{−2} frequency hertz Hz = s^{−1}

Property	Prefix	Symbol	Multiple	unit name	unit symbols
usually known as the newton, N.					
time in the combination kg m s ^{−2} . This combination is more unit of force is found by combining units of mass, length and Derived units are formed from the base units. For example, the luminous intensity candela cd current ampere A amount of substance mole mol temperature kelvin K time second s mass kilogram kg length metre m					
Quantity	SI unit	Symbol			

units in which they are measured. **SI base units:** for most quantities it is necessary to specify the Then, for example, 6859 = 6.859 × 1000 = 6.859 × 10³ and 0.0932 = 9.32 × 0.01 = 9.32 × 10^{−2}. . . .0.01 = 10^{−2} ,0.1 = 10^{−1} , . . . ,100 = 10² ,1000 = 10³ , is usually a number between 1 and 10. We make use of concisely. Each number is written in the form *a* × 10^{*n*} where *a* **Scientific notation:** is used to express large or small numbers

Units & Conversions

The Greek alphabet

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

Physical constants

Avogadro constant	<i>N</i> _A = 6.022 × 10 ²³ mol ^{−1}
Boltzmann constant	<i>k</i> _B = 1.381 × 10 ^{−23} J K ^{−1}
Planck constant	<i>h</i> = 6.626 × 10 ^{−34} J s
Elementary charge	<i>e</i> = 1.602 × 10 ^{−19} C
Ideal gas constant	<i>R</i> = 8.314 J K ^{−1} mol ^{−1}
Vacuum permittivity	<i>ε</i> ₀ = 8.854 × 10 ^{−12} J ^{−1} C ² m ^{−1}
Speed of light (vacuum)	<i>c</i> = 2.998 × 10 ⁸ m s ^{−1}
Faraday constant	<i>F</i> = <i>e N</i> _A = 96.485 kC mol ^{−1}

General Thermodynamics

First Law: For a closed system, Δ*U* = *q* + *w*. Here Δ*U* 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

=
(

∂
U

∂
T

)

V

 Heat capacity at constant pressure:

C

p

=
(

∂
H

∂
T

)

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: Δ*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* − *T**S*. **Gibbs energy:** *G* = *H* − *T**S*. **Change in Gibbs energy:** Δ*G* = Δ*H* − *T*Δ*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:**

∂

∂
T

(

∂
G

∂
T

)

p

=
−

Δ
H

T

2

.

perature at a phase boundary. Here Δ*H* = molar enthalpy of vaporisation. This equation relates the natural logarithm of the vapour pressure to the tem-

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

with gradient

−

Δ
H

R

{\displaystyle -{\frac {\Delta H}{R}}}

. (Here, *p*^o = any standard pressure). pure liquids, plotting ln

p

o

{\displaystyle p^{o}}

 against

1

T

{\displaystyle 1/T}

 produces a straight line vapour pressure for various temperatures produces a curve. For Clapeyron equation for a liquid-vapour phase boundary. Plotting Clausius-Clapeyron equation is an approximation of the

Here Δ*H* = molar enthalpy of transition, Δ*V* = change in molar volume during transition.

$$\frac{dP}{dT} = \frac{J\Delta V}{H\Delta L}$$

Clapeyron equation at a phase boundary. The slope of the phase temperature at a phase boundary. The slope of the phase in relates change in pressure to change in

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

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

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

between molecules and interparticle attractions:

Van der Waals equation takes into account the finite distance we obtain the ideal gas law.

V

m

B

{\displaystyle {\frac {V_m}{B}}}

 and

V

m

C

{\displaystyle {\frac {V_m}{C}}}

 become increasingly less important, and in the limit Observe that when the molar volume is very large, the terms *V*_{*m*} =

n

V

{\displaystyle nV}

 = molar volume, *B*, *C* etc are the **virial coefficients**.

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

because it takes into account intermolecular forces.

Virial equation of state: This improves the perfect gas law **Combined Gas Laws:**

p

1

V

1

p

2

V

2

{\displaystyle {\frac {p_{1}}{p_{2}}}={\frac {V_{1}}{V_{2}}}}

.

Perfect Gas Law: *pV* = *nRT* where *H* = ideal gas constant. of all the gases, *p*_{total}.

by multiplying the gas mole fraction, *x*_{*i*}, by the total pressure The partial pressure, *p*_{*i*}, of one of the gases can be calculated

p

t
o
t
a
l

=

p

1

+

p

2

+
⋯
+

p

n

{\displaystyle p_{total}=p_{1}+p_{2}+\dots +p_{n}}

 or each would exert if they were alone in the same volume:

exerted by a mix of ideal gases is the sum of the partial pressures **Dalton's Law of partial pressures:** states that the pressure

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

∗

{\displaystyle 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* =

∑

i

n

i

V

m
,
i

{\displaystyle \sum _{i}n_{i}V_{m,i}}

, where

*V*_{*m,i*} is the partial molar volume of the *i*th 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*} *μ*_{*A*} + *n*_{*B*} *μ*_{*B*}. More generally, with mixtures of several substances *G* =

∑

i

n

i

μ

i

{\displaystyle \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 ^o, as in *G*^o.

Reaction Gibbs energy:

Δ

r

G
=

Δ
G

Δ
ξ

{\displaystyle \Delta _{r}G={\frac {\Delta G}{\Delta \xi }}}

 is the slope of the graph of Gibbs energy against the progress of the reaction. Here, Δξ = Δ*n*_{*J*}/*ν*_{*J*} for all species *J* in the reaction. Reaction Gibbs energy at any composition of the reaction mixture can be written

$$\Delta _{r}G = \Delta _{r}G^{\circ } + RT \ln Q \quad \text{where } Q = \prod _{j}a_{j}^{\nu _{j}}$$

where *a*_{*J*} is the activity of species *J* and *ν*_{*J*} is its stoichiometric number.

At equilibrium *Q* = *K*, Δ_{*r*}*G* = 0 and −Δ_{*r*}*G*^o = *RT* ln *K* where

$$K = \prod _{j}(a_{j}^{\nu _{j}})_{\text{equilibrium}}$$

van't Hoff equation:

d

d
T

ln
⁡
K
=

Δ

r

H

o

R

T

2

.

{\displaystyle {\frac {d}{dT}}\ln K={\frac {\Delta _{r}H^{o}}{RT^{2}}}.}

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

Vectors

If **r** = *x***i** + *y***j** + *z***k** then |**r**| =

√

x

2

+

y

2

+

z

2

{\displaystyle {\sqrt {x^{2}+y^{2}+z^{2}}}}

.

Scalar product:

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

If **a** = *a*₁**i** + *a*₂**j** + *a*₃**k** and **b** = *b*₁**i** + *b*₂**j** + *b*₃**k** then

$$\mathbf {a} \cdot \mathbf {b} = a_{1}b_{1} + a_{2}b_{2} + a_{3}b_{3}$$

Vector product:

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

ê is a unit vector perpendicular to the plane containing **a** and **b** in a sense defined by the right hand screw rule.

If **a** = *a*₁**i** + *a*₂**j** + *a*₃**k** and **b** = *b*₁**i** + *b*₂**j** + *b*₃**k** then

$$\begin{aligned} \mathbf {a} \times \mathbf {b} &= (a_{2}b_{3} - a_{3}b_{2})\mathbf {i} + (a_{3}b_{1} - a_{1}b_{3})\mathbf {j} + (a_{1}b_{2} - a_{2}b_{1})\mathbf {k} \\ &= \begin{vmatrix} \mathbf {i} & \mathbf {j} & \mathbf {k} \\ a_{1} & a_{2} & a_{3} \\ b_{1} & b_{2} & b_{3} \end{vmatrix} \end{aligned}$$

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

e

−

E

a

/
(
R
T
)

{\displaystyle k=Ae^{-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

$$\ln \frac{k}{k^{\circ }} = \ln \frac{A}{k^{\circ }} - \frac{E_{a}}{RT}$$

where *k*^o 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 <i>k</i>
0	 d [A] d t = −<!-- − --> k {\displaystyle {\frac {d[A]}{dt}}=-k} 	[A] ₀ − [A] = <i>kt</i>	 [A] 0 2 k {\displaystyle {\frac {[A]_{0}}{2k}}} 	mol dm ^{−3} s ^{−1}
1	 d [A] d t = −<!-- − --> k [A] {\displaystyle {\frac {d[A]}{dt}}=-k[A]} 	[A] = [A] ₀ e ^{−<i>kt</i>}	 ln ⁡<!-- ⁡ --> 2 k {\displaystyle \ln 2/k} 	s ^{−1}
2	 d [A] d t = −<!-- − --> k [A] 2 {\displaystyle {\frac {d[A]}{dt}}=-k[A]^{2}} 	 1 [A] −<!-- − --> 1 [A] 0 = k t {\displaystyle {\frac {1}{[A]}}-{\frac {1}{[A]_{0}}}=kt} 	 1 k [A] 0 {\displaystyle {\frac {1}{k[A]_{0}}} 	mol ^{−1} dm ³ s ^{−1}
2*	 d [A] d t = −<!-- − --> k [A] [B] {\displaystyle {\frac {d[A]}{dt}}=-k[A][B]} 	 1 [B] 0 −<!-- − --> 1 [A] 0 ln ⁡<!-- ⁡ --> [B] [A] [B] 0 [A] 0 = k t {\displaystyle {\frac {1}{[B]_{0}}-{\frac {1}{[A]_{0}}}\ln {\frac {[B][A]}{[B]_{0}[A]_{0}}}}=kt} 	-	mol ^{−1} dm ³ s ^{−1}

(* A + B → P reaction.)