Appendix A Units and conversions

A.1 Prefixes

Here are some prefixes that are often used when writing scientific numbers.

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

Also not the unit Å(or Angstrom), often used to describe sizes of atoms, which is equal to 1×10^{-10} m.

Concentrations are sometimes measured in ppm or ppb. There are two types, either referring to mass (i.e. kg/kg) or to volume (i.e. m^3/m^3).

Where we are referring to mass it could be mass of a substance divided by mass of another substance (e.g. the abundance of gold in an ore is 2 ppm by mass). 2 ppm by mass means that to get the total mass of gold, first divide by 1 million and then multiply by the mass of the ore.

Where we are referring to volumes of gases (as in atmospheric science) it is usually the number of moles of a substance divided by the number of moles of the solute or of air, then multiplied by 1×10^6 in the case of ppm or 1×10^9 in the case of ppb. This is because 1 mole of any gas occupies the same volume, so volume and moles are equivalent units when we are talking about gases.

Appendix B **Common areas and volumes**



See http://math.about.com/library/blmeasurement.htm.



Appendix C Atomic structure, molecular weight and moles

C.1 Periodic table primer and Atomic structure

A compound is the name given to a substance that can be broken down into smaller units, other compounds, ions or constituent elements by chemical processes. Elements are the simplest form of chemical matter and cannot be broken down into simpler constituents by chemical processes. Elements consist of many of the same atom. We will use a simplified model of the atom but if you understand and remember it, this model is quite powerful at predicting the behaviour of elements and the sorts of compounds that they form.

Atoms are composed of 3 basic particles: protons, neutrons and electrons:

Particle	Mass	Charge
Proton	1 atomic unit	+1
Neutron	1 atomic unit	0
Electron	negligible (0)	-1

Atoms are electrically neutral: therefore the number of electrons must balance the number of protons. The simplest atom therefore is hydrogen which has 1 proton with 1 electron.

A very simplified (but useful) model of the atom that it is like a planet (electron) orbiting the sun (proton). The way that the atom behaves chemically is determined by the number of electrons it has, also equal to the number of protons. Therefore, which element it is, is determined by the number of protons—the so called atomic number.

- If we try and make the next atom up by adding 2 protons together, it doesnt work since the protons repel each other. Nuclear 'glue needs to be added by neutrons.
- All atoms heavier than hydrogen have a nucleus which is composed of neutrons and protons and a number of electrons 'orbiting the nucleus.
- The mass of the atom determined *mainly* by the number of neutrons and protons (the mass of electrons is negligible compared to neutrons and protons).

Nomenclature:

The number of protons (=number of electrons) uniquely determines what sort of element that an atom is but (within limits) the number of neutrons can be different for different atoms of the same element—thus giving different *isotopes* of the element.

The mass of the proton is so small on our scale of things that we need some way of talking about sensible quantities—you wont burn 1 atom of hydrogen, you will



burn a few grams or kilograms—so we can ask: how many hydrogen atoms, *Z*, are there in 1g?

$$N_A \times 1.66 \times 10^{-24} = 1 \text{ gram}$$

(Number of atoms in 1 gram) × (mass of 1 H atom) = 1 gram

Rearranging we find that $N_A = 6.02 \times 10^{23}$. This is a special number known as *Avogadros Number*.

We may think of it as a factor that scales between atomic sizes and quantities with which we can deal. It is equal to 6.02×10^{23} atoms or molecules and called a mole. 1 mole of any substance contains 6.02×10^{23} atoms or molecules.

If we think of helium which has 2 protons and 2 neutrons, so the helium atom has a mass of $4x1.66 \times 10^{-24}$ g or, equally, 1 mole of helium atoms weighs 4 grams.

 238 U is atomic number 92 and mass 238 so it has 92 protons and 146 neutrons or the mass of the uranium atom is $238 \times 1.66 \times 10^{-24}$ g, or equally, 1 mole of uranium atoms weighs 238 grams.

WebElements: the periodic table on the world-wide web

www.webelements.com

1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
hydrogen																		helium
1																		2
н																		He
1.0079		Key:												· ·		n		4.0026
lithium 2	beryllium			ate	element name	e hor							boron	carbon	nitrogen	oxygen g	fluorine	neon 10
				att									Ē	ŏ		Ö	<u> </u>	
LI	Ве	symbol											В	C	N	U		Ne
6.941	9.0122		atomic weight (mean relative mass)											12.011	14.007	15.999	18.998	20.180
sodium	magnesium												aluminium	silicon	phosphorus	sulfur	chlorine	argon
11	12														15	16	17	18
Na	Mg		AI SI P S CI A														Ar	
22.990	24.305												26.982	28.086	30.974	32.065	35.453	39.948
potassium	calcium		scandium	titanium	vanadium	chromium	manganese	iron	cobalt	nickel	copper	zinc	gallium	germanium	arsenic	selenium	bromine	krypton
19	20		21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
K	Ca		Sc	Ti	V	Cr	Mn	Fe	Со	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
39.098	40.078		44.956	47.867	50.942	51.996	54.938	55.845	58.933	58.693	63.546	65.38	69.723	72.61	74.922	78.96	79.904	83.80
rubidium	strontium		yttrium	zirconium	niobium	molybdenum	technetium	ruthenium	rhodium	palladium	silver	cadmium	indium	tin	antimony	tellurium	iodine	xenon
37	38		39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
Rb	Sr		Y	Zr	Nb	Мо	Тс	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те		Xe
85.468	87.62		88.906	91.224	92.906	95.96	[98]	101.07	102.91	106.42	107.87	112.41	114.82	118.71	121.76	127.60	126.90	131.29
caesium	barium		lutetium	hafnium	tantalum	tungsten	rhenium	osmium	iridium	platinum	gold	mercury	thallium	lead	bismuth	polonium	astatine	radon
55	56	57-70	/1	72	73	74	75	76	11	78	79	80	81	82	83	84	85	86
Cs	Ba	*	Lu	Hf	Та	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
132.91	137.33		174.97	178.49	180.95	183.84	186.21	190.23	192.22	195.08	196.97	200.59	204.38	207.2	208.98	[209]	[210]	[222]
francium	radium		lawrencium	rutherfordium	dubnium	seaborgium	bohrium	hassium	meitnerium	darmstadtium	n roentgenium	ununbium	ununtrium	ununquadium	ununpentium	ununhexium	ununseptium	ununoctium
87	88	89-102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
Fr	Ra	**	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo
[223]	[226]		[262]	[267]	[268]	[271]	[272]	[270]	[276]	[281]	[280]	[285]	[284]	[289]	[288]	[293]	- 1	[294]

	lanthanum	corium	praceodymium	noodymium	promothium	comorium	ouropium	aadolinium	torbium	dyeprosium	holmium	orbium	thulium	vttorbium
			praseouymum	neouymium	prometinum	Samanum	europium	gauoimium	leibiuiii	uyspiosium	nonnunn	erbium		yllerblum
	57	58	59	60	61	62	63	64	65	66	67	68	69	70
						0								
*lanthanoids	Ia		Pr	NO	Pm	Sm			ID		HO	– r	Im	YD
lantinanoido	Lu							U u		_y				
	138.91	140.12	140.91	144.24	[145]	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.06
	actinium	thorium	protactinium	uranium	neptunium	plutonium	americium	curium	berkelium	californium	einsteinium	fermium	mendelevium	nobelium
	89	90	91	92	93	94	95	96	97	98	99	100	101	102
**actinoide	٨c	Th	Da	11	Nn	Du	Δm	Cm	RL	Cf	Ec	Em	Md	No
actinoius	AC		Га	U	N	ГU	AIII	GIII	DR	G	LJ			INU
	[227]	232.04	231.04	238.03	[237]	[244]	[243]	[247]	[247]	[251]	[252]	[257]	[258]	[259]

Symbols and names: the symbols and names of the elements, and their spellings are those recommended by the International Union of Pure and Applied Chemistry (IUPAC - http://www.iupac.org/). Names have yet to be proposed for the most recently discovered elements beyond 112 and so those used here are IUPAC's temporary systematic names. In the USA and some other countries, the spellings **aluminum** and **cesium** are normal while in the UK and elsewhere the common spelling is **sulphur**. Group labels: the numeric system (1–18) used here is the current IUPAC convention.

Atomic weights (mean relative masses): Apart from the heaviest elements, these are the IUPAC 2007 values and given to 5 significant figures. Elements for which the atomic weight is given within square brackets have no stable nuclides and are represented by the element's longest lived isotope reported at the time of writing.

©2007 Dr Mark J Winter IWebElements Ltd and University of Sheffield. webelements@sheffield.ac.ukl. All rights reserved. For updates to this table see http://www.webelements.com/nexus/Printable Periodic Table (Version date: 21 September 2007).

C.2 Bonding and Stoichiometry

In building up heavier and heavier atoms more protons, neutrons and electrons are added, but electrons add into *shells*. First shell contains 2 electrons, successive shells contain 8 (and higher up the periodic table, 10+8). The sequence is 2, 8, 8, 18, 18, 32, 32,...

So in going from helium (2 electrons) to lithium (3 electrons) the third electron starts a new shell and is much more loosely held to the nucleus—therefore it is easier to remove so lithium is chemically reactive—it is relatively easy for it to lose an electron to form an ion, Li⁺.

As we go through Li, Be, B, C, N, O, F we finally get to Ne which has 8 electrons in its outer shell and this is complete—its very difficult to add or take away electrons from neon so it is chemically unreactive. Fluorine has 7 electrons in its outer shell if it can grab an electron it will have a full shell and will do so if possible—so fluorine is very reactive and will make an F^- ion if it can. So if we react Li with F, fluorine will grab the electron from Li - both will have closed shells and be most stable—so lithium and fluorine will react in a 1:1 ratio. They are bonded together *ionically* since the formation of the compound involves the transfer of electrons from one atom to the other. The energy that it takes to remove an electron from an atom is called the ionization potential, the energy released by an atom in capturing an electron called the electronegativity.

Oxygen has 6 electrons in its outer shell so requires 2 electrons to fill the shell. If we burn Li in oxygen we will require 2 Li atoms to each oxygen so forms a compound Li₂O. Mg has 2 electrons in its outer shell. It is easier for it to lose the 2 electrons to create a complete shell than to gain 6 so Mg forms a Mg^{2+} ion and will form the compound MgO or MgF_2 .

In the middle of the periodic table e.g. carbon, which has 4 electrons in its outer shell, atoms can either lose 4 or gain 4 electrons. Neither option is easy so carbon tends to form another sort of bond, a *covalent* bond. In this type of bonding the electrons are shared between atoms so that at least some of the time the shells of each atom is filled. This type of bonding also occurs when 2 or more atoms are the same, eg F_2 or O_2 .

Using this very simple model we can account for and predict how most of the elements are arranged in the periodic table and how they will react with other elements.

Elements will thus react with each other in relatively simple ratios—this is called *stoichiometry*. We can write equations which describe how elements and compounds react together. To balance these reactions we must balance the number of atoms of each element and charges. Atoms react in simple atomic ratios, but since they weigh very different amounts, e.g. $H_2 + O \rightleftharpoons H_2O$ (H= 1, O= 16), it follows that 2 unit masses of hydrogen will react with 16 unit masses of oxygen. The masses of atoms are extremely small and the simplest, the hydrogen atom which is simply a proton and an electron has a mass of 1.66×10^{-27} kg or 1.66×10^{-24} g.

In most of the chemical reactions that we meet, atoms react together in simple ratios (like lithium and oxygen and other examples we met before). This is because they react as atoms but the masses that react are very different because the atoms weigh different amounts.

C.3 Balanced equations

Chemical reactions are described by chemical equations which show how the different atoms and molecules react with each other.

e.g. a particularly simple case is hydrogen burns in oxygen to make water

$$H_2 + O \rightleftharpoons H_2 O$$

A *balanced equation* accurately describes how many atoms and molecules of each type react together. The rules are fairly straightforward for balancing equations:

- Charge must balance on both sides of the equation
- Look at the cations (e.g. Ca, Mg, Na etc) which only occur in one molecule or in one form on one side of the equation and balance these.
- Repeat the process for other cations (Si, Al)
- Balance the rarer anions (e.g. S, P, C)
- Balance the abundant anions, (H, O)

So, faced with the reaction; ferric chloride reacts with ammonium hydroxide to make ferric hydroxide plus ammonium chloride we have the initial, unbalanced equation:

$$FeCl_3 + NH_4OH \rightleftharpoons Fe(OH)_3 + NH_4Cl$$

Balance cations:

$$\therefore FeCl_3 + NH_4OH \rightleftharpoons Fe(OH)_3 + NH_4Cl$$

Balance rarer anions (Cl)

$$\therefore FeCl_3 + NH_4OH \rightleftharpoons Fe(OH)_3 + 3NH_4Cl$$

Balance abundant anions

$$\therefore FeCl_3 + 3NH_4OH \rightleftharpoons Fe(OH)_3 + 3NH_4Cl$$

following each step above and the equation is now balanced.

C.4 Ideal gas law

Pressure is a force per unit area. For example a 102 g mass placed on a horizontal plane of glass on earth exerts a pressure of 1 Pa on the plane of glass.

C.4.1 Basic law

The ideal gas law was first derived empirically by combining both Boyle's law and Charles' law (see http://en.wikipedia.org/wiki/Ideal_gas_law). It can be stated as:

$$PV = NRT$$
 (C.1)

where *P* is the gas pressure, *V* is the volume of the gas, *N* is the number of moles of gas, R = 8.314 [Pa m⁻³ mole⁻¹ K⁻¹] is the universal gas constant and *T* is the temperature.

C.4.2 Partial pressure

In a container with several gases one often refers to each of the gases having a 'partial pressure'. This is the pressure (force per unit area on the container) that each gas individually exerts. The total pressure is just the sum of partial pressures $P = p_1 + p_2 + ...$, where p_1 is the partial pressure of gas component 1 and p_2 is the partial pressure of component 2. Each component therefore obeys:

$$p_i = \frac{N_i RT}{V} \tag{C.2}$$

where p_i is the partial pressure of component *i* and N_i is the number of moles of component *i*.

When we use the units of parts-per (e.g. parts per million or parts per billion) we are referring to the volume that a gas component would take up at the same total pressure as the mixture divided by the volume of the mixture. This turns out to be the ratio of the two pressures (i.e. the partial pressure and the total pressure) as everything else cancels:

$$\frac{p_i}{P} = \frac{N_i}{N} \tag{C.3}$$

which is also the ratio of the number of moles of component i and the total number of moles. For example the abundance of oxygen in earth's atmosphere is the ratio of the number of moles of oxygen to the number of moles of air.

C.5 Acids and bases

Note that to calculate the pH of an acid use the formula:

$$pH = -\log_{10}[H^+]$$
(C.4)

where $[H^+]$ is the concentration of H^+ ions in solution in moles per litre.

Usually the solution is water and water supplies its own concentration of H^+ . The amount can be calculated using the fact that the pH of water is 7 so

$$7 = -\log_{10}[H^+] \tag{C.5}$$

$$10^{-7} = [H^+] \tag{C.6}$$

APPENDIX C. ATOMIC STRUCTURE, MOLECULAR WEIGHT AND MOLES10

So water contains 10^{-7} moles per litre of $[H^+]$ ions.

Appendix D Energy, Heat and Power

Thermodynamics is primarily the study of energy and its interaction with matter. Energy can take many forms: the energy an object has by virtue of its motion is called kinetic energy; the kinetic energy of molecules moving randomly is called heat energy; the energy required to lift or shove an object that is acted on by such forces as gravity and friction is called work; the energy available for release by dropping an elevated object is called potential energy; the energy available for release by burning substances such as coal is called chemical energy; and chemical energy, when released, often takes the form of heat energy.

The ways energy can interact with matter are likewise numerous. Energy can warm matter, melt it, freeze it, boil it, expand or contract it, scramble or unscramble it, or mutate it. The results depend on what kinds of energy and matter are involved. Despite the apparent complexity, however, a few simple and universal physical laws have been discovered that allow us to make sense of the whole story. Among these are the laws of thermodynamics. The first law states that the total amount of energy in a dosed system (i.e., one which energy cannot enter or leave) remains constant, regardless of the transformations among energy types within the system. This law plays a central role in modeling both meteorological phenomena and physiological aspects of animal interactions with their environment. The second law, which describes constraints on the conversion of one type of energy to another, is particularly useful for evaluating the performance of technological devices designed to convert one form of energy to another.

The SI units of energy (and heat) is the joule (J), which is the energy required to lift a mass of 102 g (on earth) 1 metre in height.

D.1 Heat capacity

Heat is a form of energy and can also be measured in joules. It relates the amount of heat applied to some matter to a measured temperature rise. Usually the change is assumed to occur at a constant volume or pressure (if in a gas). For this course we just consider changes occuring in solids or liquids, which generally occur at a constant volume. An equation linking heat to temperature change is therefore:

$$Q = m \times C \times \Delta T \tag{D.1}$$

where Q is the amount of heat energy absorbed by the solid, m is the mass of the substance, C is the heat capacity of the substance (measured in Jkg⁻¹K⁻¹) and ΔT is the change in temperature. Each substance has it its own heat capacity.

D.2 Latent heat

When substances change phase energy is required to create order within the arrangement of molecules. E.g. ice is more ordered than liquid water because of the additional bonds, liquid water is more ordered than water vapour due to hydrogen bonding. As an example consider boiling a kettle full of water; as you put heat into the water the temperature of the water will change (in accord with the heat capacity), once the liquid water gets to 100°C the energy that is added to the water will go into breaking the hydrogen bonds, the phase change is assumed to occur at constant temperature. an equation relating the heat input required for the phase change is:

$$Q = \Delta m \times L \tag{D.2}$$

where Q is the heat input, Δm is the mass turned into the other phase, and L is the latent heat of phase change (Jkg⁻¹).

D.3 Power

This is defined as the rate of energy transfered and measured in joules per second $(J s^{-1})$. The unit J s⁻¹ is also called a watt (W). As an example going back to the kettle: a kettle could supply the required amount of heat, Q, to boil the liquid water in 1 minute or within 2 minutes. In the first case the kettle power is Q/60, whereas in the second case the kettle power is Q/120, so it is half as powerful. The same amount of total energy is supplied in both cases.

D.4 Potential energy

This is stored energy, or energy that has the potential to do something. Usually when we talk about this kind of energy we think about objects a certain height above the ground. In this case the objects potential energy is:

$$PE = mg\Delta h \tag{D.3}$$

where *m* is the objects mass, *g* is the acceleration due to gravity and Δh is the height the object would fall before hitting the ground. Also note that in the absence of forces other than gravity *PE* is equal to the work done in lifting a mass a height Δh against gravity: a consequence of the work-energy equivalence theorem.

D.5 Kinetic energy

This is energy associated with a moving mass. It is equal to:

$$KE = \frac{1}{2}mv^2 \tag{D.4}$$

where *m* is the mass and *v* is its speed (m s⁻¹).

D.6 Conservation of energy

Energy cannot be created or destroyed, but only changed from one type to another. In our case of a mass a distance Δh above the ground, if we were to drop this mass and allow it to fall, the potential energy would be transferred into kinetic energy as the object moves toward the ground. At the point when it hits the ground it will have maximum kinetic energy and no potential energy (measured from above the ground). Therefore we can write:

$$mg\Delta h = \frac{1}{2}mv^2 \tag{D.5}$$

or

$$v = \sqrt{2g\Delta h} \tag{D.6}$$

Once it hits the ground some of this kinetic energy may be transferred into heat and go into changing the temperature of the object (due to specific heat capacity), some will also heat the ground and some will be changed into sound energy (or kinetic energy of the air).

D.7 Carnot efficiency

This is the maximum theoretical efficiency that a heat engine, heat pump or power station can operate at. It is never reached in practice. Note that a heat pump extracts the heat energy from a warm substance (usually hot air or steam) by forcing the warm substance to do some form of work. Once the hot steam has done the work it leaves the system cooler than before (as the kinetic energy of molecules has been transferred to the turbine). From the equation for heat capacity the amount of heat energy extracted is:

$$Q = mC(T_H - T_C) \tag{D.7}$$

The theoretical maximum amount of heat than can be extracted is the amount of heat we could extract if we cooled the substance to absolute zero when extracting heat or:

$$Q_{max} = mC(T_H - 0) \tag{D.8}$$

The ratio of these is the efficiency of the heat pump:

$$\epsilon = \frac{\mathcal{MC}(T_H - T_C)}{\mathcal{MC}(T_H - 0)} = \frac{T_H - T_C}{T_H}$$
(D.9)

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