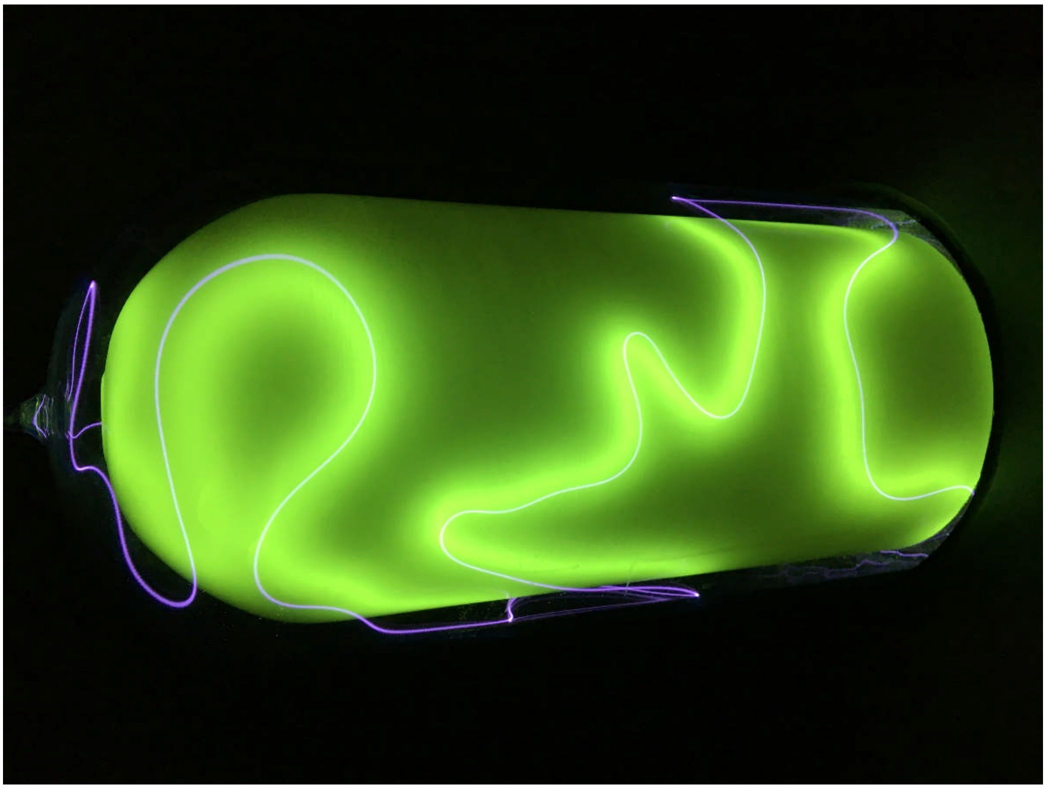
UNIVERSITY OF LEEDS



UNDERSTANDING CHEMISTRY IN A PHYSICS CONTEXT

Written by Sukhjivan Sandhu

School of Physics and Astronomy

University of Leeds

2018

TABLE OF CONTENTS

INTRODUCTION

In order to investigate anecdotal feedback from students, in 2017, an undergraduate student, Daniel Swindlehurst, in the School of Physics and Astronomy at the University of Leeds undertook a final year project investigating the link between students' A-level subjects and their success in a Physics degree. Confirming suspicions from the initial feedback, there was a link between whether students had A-level Chemistry and their attainment in some level one modules core Physics modules. This attainment gap disappeared in later years.

To address this issue, in 2018 a student intern was recruited to create a resource to support those students without A-level chemistry that were taking a Physics degree. This resource was based on the relevant aspects of A-level chemistry courses, and was wholly authored by a 2nd year Physics student, Sukhjivan Sandhu, with direction provided by Dr Samantha Pugh, an academic in the School.

One of the best features of the resource being student-authored is that it is written in a different style to a standard text book. There is a much more informal and conversational tone, whilst simultaneously ensuring that there is rigour in the content.

The resource was trialled with undergraduate students; it was highlighted as extremely valuable for those without A-level Chemistry, and an excellent recap for everyone else. The resource was made available through our Virtual Learning Environment and promoted by course tutors and our Peer Mentors.

We hope that this resource will be useful in the learning of core physics at undergraduate level, particularly where students do not have a background in A-level Chemistry.

Dr Samantha Pugh
School of Physics and Astronomy
University of Leeds
Leeds LS2 9JT
s.l.pugh@leeds.ac.uk

1. THE ATOM

1.1: SUBATOMIC PARTICLES

I am sure you are all very familiar with the atom, however to ensure that nothing is skipped over I will be covering it anyway. Atoms are made up of 3 main subatomic particles: Protons, Neutrons and Electrons.

Subatomic Particle (representative symbol)	*Relative Charge*	*Relative Mass*
Proton (p or e^+)	+1	1
Neutron (n)	0	1
Electron (e^-)	-1	1/2000

NB: The charge and mass are relative and therefore have no units.

Figure 1: Table to show basic properties of subatomic particles

As you can see in figure 1, protons and electrons have equal and opposite charge. Due to what is called the ***electrostatic force of attraction*** or the ***Coulomb force***, these two subatomic particles are attracted to one and other. It is important to remember that opposite charges attract whilst like charges repel, and it is also important to note that any stable atom has the same number of protons and electrons (to keep its overall charge neutral).

Example 1: *If a proton and a neutron were next to each other, would there be an electrostatic force of attraction between them?*

Example 2: *If there was a proton and an electron next to each other, would there be a Coulomb force between them? If so, would it be an attractive or repulsive force?*

Key Definitions:

- Electrostatic force of attraction – where objects with opposite charge are attracted to one another (the attractive version of the Coulomb force).
- Coulomb force – the force exerted by a stationary charge on another stationary charge, where the strength of the force is defined by Coulomb's Law.

1.2: THE ATOMIC MODEL

The atomic model has taken many forms throughout history, but the most important one to worry about for now is the Bohr Model of the atom which was introduced by Niels Bohr and Ernest Rutherford in 1913. The Bohr Model is not a perfect model and later during your time doing Physics in Leeds you will come across quantum mechanical models of the atom, however despite not being perfect we can still learn a lot from it.

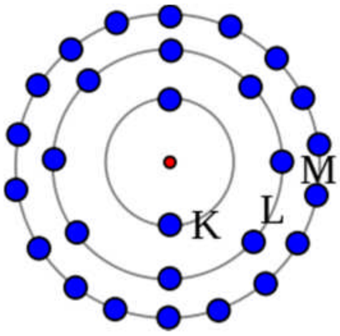


Figure 2: A diagram to show the Bohr Model of the atom. [1]

1.2A: The Nucleus

At the centre, the red dot represents what is known as the ***nucleus***, and as you can see the nucleus is clearly a very small part of the overall atom. The nucleus consists of protons and neutrons, also known as ***nucleons***, however you will have hopefully noticed a slight problem. If you remember from the subatomic particles section, we know that protons have a relative charge of +1, and we also know that like charges repel each other due to the Coulomb force. For protons to all be packed into such a tight area there must be a force even stronger than the coulomb force that works over short distances, and that is known as the ***nuclear strong force***. We are not going to talk much about it, but it is important you know it exists and that it explains why the protons can be so close together. The other important thing to note is that most of the mass of the atom is concentrated in the nucleus, as the nucleons are the heaviest subatomic particles.

Example 3: Is an electron a nucleon?

Example 4: How do protons overcome the repulsive Coulomb force between them inside the nucleus and manage to stay so close to each other?

Key Definitions:

- Nucleus – the positively charged central core of an atom, consisting of protons and neutrons and containing nearly all its mass.
- Nucleons – the subatomic particles that reside in the nucleus, protons and neutrons.
- Nuclear strong force – the strongest of the four most basic forces in nature, responsible for holding the nucleons together.

1.3: ELECTRONIC STRUCTURE

1.3A: BOHR MODEL

From the Bohr Model in figure 2 we can see some important features of the electrons (blue dots) in the atom. We can see that the inner shell can only hold 2 electrons whilst the outer 2 shells can hold 8, to explain this we need to delve a little deeper:

1. The electrons can only exist in what we call ***electron shells***, the electrons cannot exist anywhere else.
2. The shells have their own fixed energy.
3. Electrons can move between shells, but this would cause a change in energy. The change in energy is accounted for by electromagnetic radiation (usually a gamma ray being absorbed or emitted).

Key Definitions:

- Electron shells – can be thought of as an orbit followed by electrons around an atom's nucleus.

1.3B: SHELLS, SUB-SHELLS AND ORBITALS

Despite the Bohr model claiming that each shell has its own fixed energy, it was later found that two electrons in the same shell can have different energies, so we need a new way to think about shells. It was then decided that shells must be made up of ***sub-shells*** and ***orbitals***.

In chemistry the sub-shells are labelled s, p, d, f, … (you will not need any more than this) and they each hold a certain number of orbitals – each orbital can hold 2 electrons. Sub-shell s has just one orbital, therefore it can hold just 2 electrons, sub-shell p has 3 orbitals and can hold 6 electrons, d has 5 orbitals and can hold 10 electrons whilst f has 7 orbitals and can hold 14 electrons. As you move up one shell, you gain 2 new orbitals, hence 4 new electrons. This is very important to know so take your time and go over it again until you understand, figure 3 may help things seem a bit clearer.

Shell	*Sub-Shells*	*Total Number of Orbitals*	*Total Number of Electrons in Shell*
1	s	1	2 = 2 electrons
2	s, p	1 + 3 = 4	2 + (3 x 2) = 8 electrons
3	s, p, d	1 + 3 + 5 = 9	2 + (3 x 2) + (5 x 2) = 18 electrons
4	s, p, d, f	1 + 3 + 5 + 7 = 16	2 + (3 x 2) + (5 x 2) + (7 x 2) = 36 electrons

Figure 3: A table to show shells, sub-shells and orbitals and hence how many electrons the shells can hold

To recap, we now have shells, which are made up of sub-shells, which contain orbitals, which hold the electrons. Got it? Now it is time to find out why this happens by looking at quantum numbers.

Example 5: How many electrons can an orbital hold?

Example 6: How many more electrons can sub-shell f hold than sub-shell s?

Key Definitions:

- Sub-shells – a subdivision of an electron shell, a sub-shell contains a specific number of orbitals that house electrons.
- Orbital – an area od space that can contain up to two electrons at a time, one spin-up and one spin-down.

1.3C: QUANTUM NUMBERS

Shells are associated with the ***principal quantum number, n***, and can take the values 1, 2, 3, 4, … (any integer value). In the diagram above, letters are used to represent n, where K is n = 1, L is n = 2, M is n = 3, N is n = 4, and so on. I will do a table below for completeness, but you do not need to worry about these letters, just stick to the numbers. All electrons on a shell will have the same principal quantum number, and as the principal quantum number increases, the electrons on it are further away from the nucleus and thus have a higher energy.

Example 7: What does the principal quantum number represent physically?

Principal Quantum Number (n)	*Letter*
1	K
2	L
3	M
4	N

Figure 4: A table to show the principal quantum numbers.

Orbital Quantum Number (l)	*Sub-Shell*
0	s
1	p
2	d
3	f

ENERGY INCREASES

Figure 5: A table to show orbital quantum numbers and how they relate to sub-shells.

Sub-Shells are associated with the ***orbital quantum number, l***, and are given values 0, 1, 2, 3, …, n-1 (where n = principal quantum number). It is important to not confuse the orbital quantum number with the orbitals as they are different things. The way the values of l relate to the sub-shells above is as follows: s is l = 0, p is l = 1, d is l = 2, f is l = 3, etc.

Example 8: *What does the orbital quantum number physically represent?*

Example 9: *How many electrons can the sub-shell that corelates to "orbital quantum number" 2 hold?*

Orbitals are associated with the ***magnetic quantum number, m_l***, and takes values from -l through to +l, where l is the orbital quantum number. I.e. this sequence of numbers would be -l, -l+1, -l+2, …, l-2, l-1, l.

Example 10: *If the orbital quantum number for a given sub-shell was 3, what would the range of values of the magnetic quantum number be? What does this range of numbers represent?*

Example 11: *If the principle quantum number for an electron was 3, what would the orbital quantum number be and what would be the range of magnetic quantum numbers?*

The reason each orbital can hold two electrons is due to a property called ***spin, m_s***, which is also a quantum number. Every electron has a spin value which is either spin-up (+1/2) or spin-down (-1/2). Even though this property is called spin, it is important to note that the electron is not actually spinning in a physical sense. It is a quantum mechanical property that you do not need to worry about much for now.

Name	*Principle Quantum Number (Shells), n*	*Orbital Quantum Number (Sub-Shells), l*	*Magnetic Quantum Number (Orbitals), m_l*	*Spin, m_s*
Rule	Integers going up from 1	n-1	-l, …, +l	+1/2 and -1/2 in each orbital
	1	0	0	2 electrons
	2	1	-1, 0, +1	6 electrons
	3	2	-2, -1, 0, +1, +2	10 electrons
	4	3	-3, -2, -1, 0, 1, 2, 3	14 electrons

Figure 6: A summary table to show every quantum number.

From figure 6 we can see clearly why when you go up the sub-shells they can each hold 4 more electrons.

Example 12: *If each electron must be in a unique quantum state, why can an orbital hold 2 electrons?*

Key Definitions:

- Principal quantum number – quantum number used to describe the state of an electron, corresponds to which shell the electron is in.
- Orbital quantum number – quantum number used to describe the state of an electron, corresponds to which sub-shell the electron is in.
- Magnetic quantum number – quantum number used to describe the state of an electron, corresponds to the number of orbitals a sub-shell has.
- Spin – quantum number used to describe the state of an electron, corresponds to either a spin-up state or a spin-down state.

1.4: THE PERIODIC TABLE

1.4A: NUCLEAR SYMBOL

$^{A}_{Z}X$ This is what is known as a ***nuclear symbol***, where X represents the element symbol, A is the ***mass number*** and Z is the ***atomic (proton) number***. Each element has its own unique element symbol, you will become familiar with these as you come across them more often. The mass number, A, is the number of protons and neutrons in the atom. The proton number, Z, is of course the number of protons. By doing a simple calculation of A-Z you can work out the number of neutrons, N, and as you already know an element has the same number of protons and electrons. Therefore, from just the nuclear symbol you can work out how many of each subatomic particle makes up the atom.

Here are some example of nuclear symbols and what elements they represent: hydrogen - $^{1}_{1}H$, deuterium - $^{2}_{1}H$, helium - $^{4}_{2}He$, lithium - $^{7}_{3}Li$, etc. Notice that hydrogen and deuterium share the same element symbol, but their nuclear symbol is different. This is because they *are* the same element, but they are ***isotopes*** of each other, which we will talk more about in the next section.

Example 13: *Using the period table below (figure 7) find: The nuclear symbol of the elements with atomic numbers of 11, 33 and 57.*

Key Definitions:

- Nuclear symbol – a notation for atoms that consists of the mass number, proton number and element symbol.
- Mass number – the total number of nucleons (protons and neutrons) in the nucleus of an atom.
- Atomic (proton) number – the total number of protons in the nucleus of an atom, tells you what element the atom is.

1.4B: ISOTOPES AND IONS

Deuterium is an ***isotope*** of Hydrogen. An isotope of an element is an atom with the same number of protons but a different number of neutrons. The same number of protons means it is the same element, and its Z does not change, but a different number of neutrons will change the mass of the atom, hence A will change. Isotopes of an element will have the same chemical properties, but they will have different physical properties. This is because chemical properties depend on the number and arrangement of the electrons, whereas physical properties depend more on the mass of the atom.

Example 14: *Do hydrogen and deuterium have the same number of: protons? electrons? neutrons? And would they chemically react in the same way?*

Any naturally occurring element will have the same number of protons and electrons so to keep its overall charge neutral, but it is possible to remove or add electrons to an element. When this happens, you create an ***ion***. We know electrons have a negative charge, therefore if we have more electrons than protons, we have a ***negative ion***, e.g. Li^{-1} would be a lithium atom with an extra electron. A ***positive ion*** must therefore have fewer electrons that protons, e.g. O^{+2} is an oxygen atom with 2 electrons taken away from it. Ions tend to form to be in accordance with the ***octet rule*** which we will look at shortly.

When creating an ion, it is important to note that you cannot just remove an electron from the inner shells, you can only add or remove electrons to the outer shells, i.e. the valence electrons. We will talk about why in the ***valence electrons*** section.

Example 15: *If a carbon atom has 11 electrons would this be an ion, and if so what charge is the ion?*

Key Definitions:

- Isotope – atoms with the same atomic number but different mass numbers, i.e. same number of protons but different number of neutrons.
- Ion – an atom with a different number of protons and electrons.
- Negative ion – an atom with more electrons than protons.
- Positive ion – an atom with more protons than electrons.
- Valence electron – electrons in the outermost shell of an atom.

1.4C: THE PERIODIC TABLE

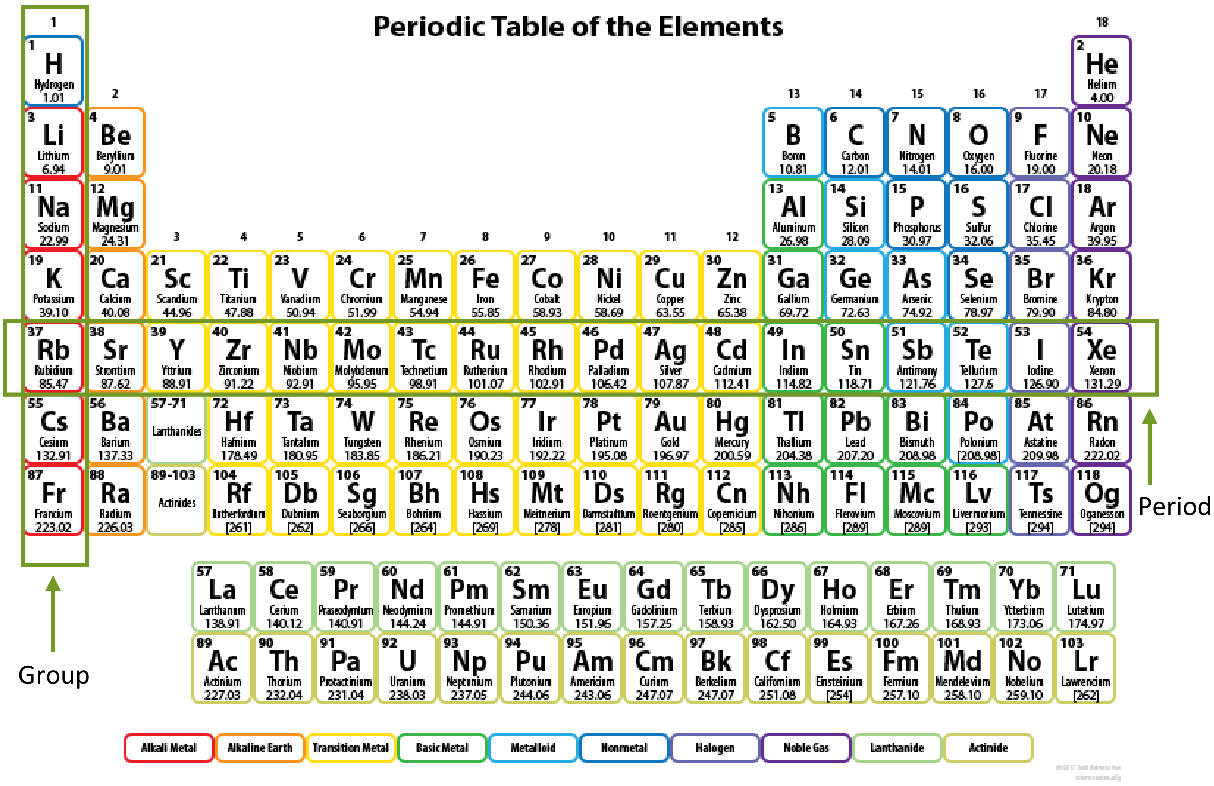


Figure 7: The Periodic Table. [2]

The elements in the periodic table are listed chronologically from top left to bottom right in terms of their proton number and can be thought of as a collection of ***groups*** or ***periods***.

A group in the periodic table goes vertically downward. The key characteristic of groups is that every element in a group has the same number of valence electrons (i.e. the same number of electrons in their outer shell). E.g. Hydrogen (H) and Potassium (K) are in group 1 and have 1 valence electron in their outer shell, Boron (B) and Aluminium (Al) are both in group 13 both have 3 valence electrons. Do not confuse them being in group 13 and having 13 valence electrons, despite that being the case for some groups it is not a rule of thumb to follow. Later we will look at another example of the periodic table to help explain why it is like this.

You can see some of the names of the groups at the bottom of figure 7, e.g. the halogen group on the right-hand side of the table, all halogens have 7 valence electrons, just one electron short of a full outer shell. The group on the far right-hand side is the noble gases, they all have a full outer shell and therefore are inert (i.e. they rarely react with other elements as they are already stable).

The noble gases conform to the ***octet rule***, a rule which states that atoms strive to fill the s and p sub-shells of their outer most shell, needing 8 electrons. Noble gases have their s and p sub-shells filled with 8 electrons in their outer shell (also considered to be a *closed shell*), therefore they do not react with other elements as they are happy and chemically stable.

A period goes horizontally across the table as you can see labelled above. All elements in a period also have something in common, they all have the same number of shells (i.e. the same principal quantum number). E.g. Hydrogen (H) and Helium (He) both only have 1 shell (the 1s orbital) and the elements in period 2 have 2 shells (1s, 2s and the 2p orbitals). Remember, the number of shells is not the same as the number of orbitals as we have just seen.

Example 16: *What do elements in the same group in the periodic table have in common?*

Example 17: *Why are the noble gases inert?*

Example 18: *What do elements in the same period in the periodic table have in common?*

Key Definitions:

- Group – a set of elements that belong to the same column in the periodic table and have similar chemical properties due to their electronic structure.
- Period – a set of elements that belong to the same row in the periodic table, they have the same principal quantum number.
- Octet rule – the striving of atoms to fill their s and p sub-shells of their outer shell, requiring 8 electrons.

1.5: ELECTRONEGATIVITY, ATOMIC RADII AND IONISATION ENERGY

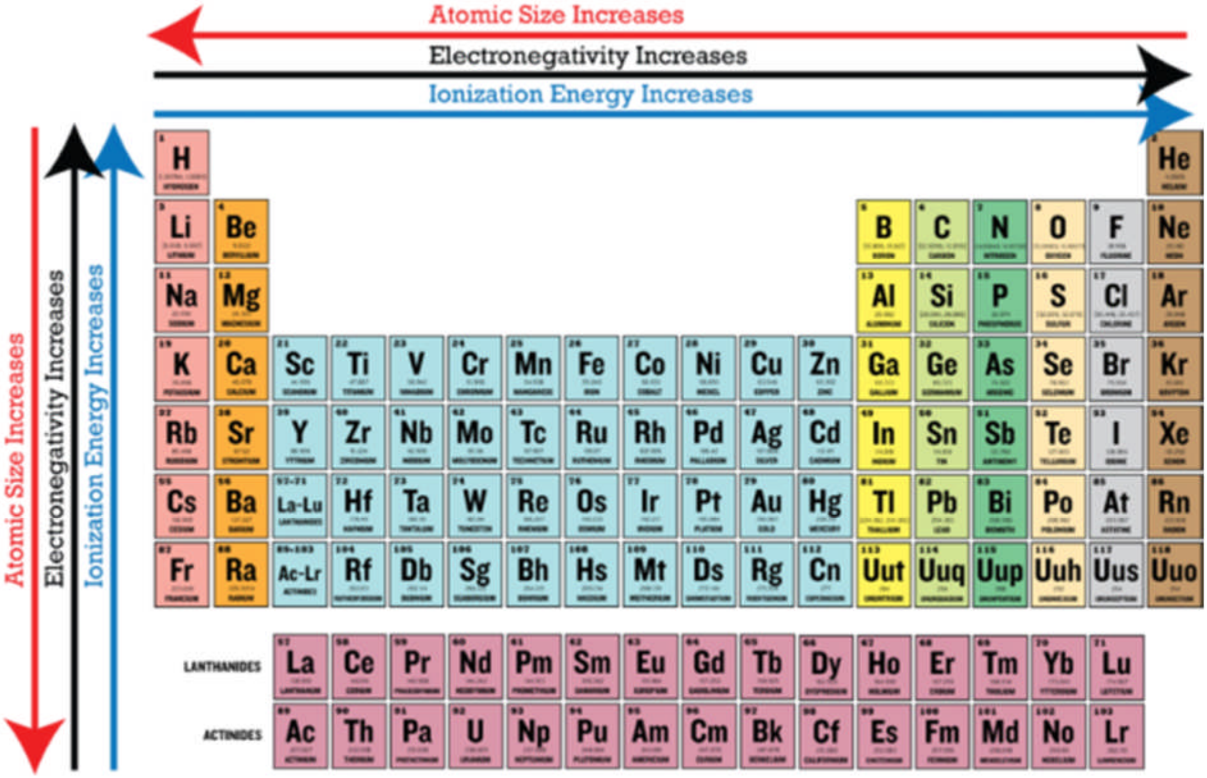


Figure 8: The Periodic Table with its periodic trends labelled. [3]

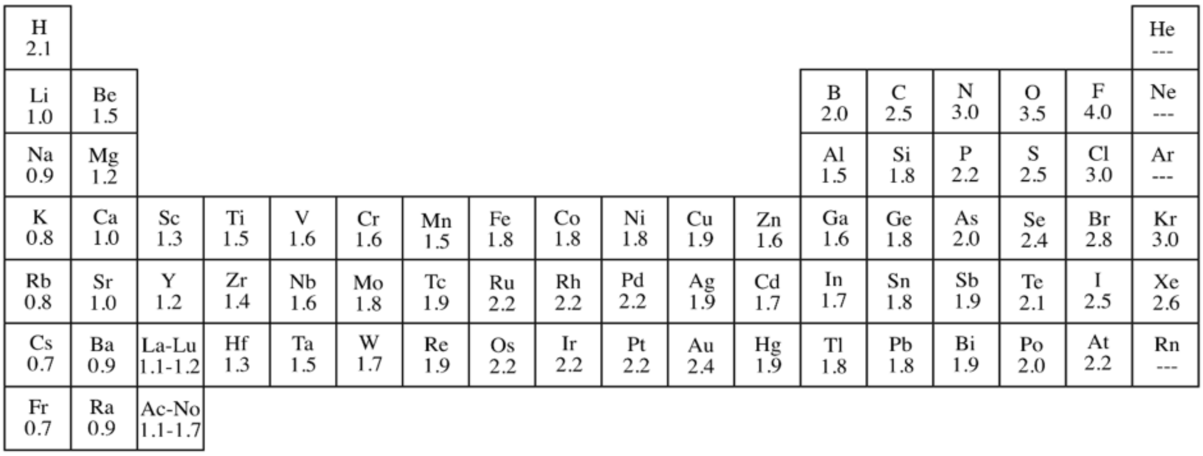
Despite the fact an element is neutral overall, we can split an atom into its oppositely charged parts. There is a Coulomb force of attraction between the positively charged nucleus of an atom and the negatively charged electrons that are orbiting it where the nucleus is essentially holding onto its electrons. An important thing to note is that Coulomb forces are inversely proportional to the distance between the two charges, therefore as the charges move further away, the force between them weakens.

1.5A: ELECTRONEGATIVITY

Electronegativity is an atoms ability to attract electrons towards it, or inversely ***electropositivity*** is an atoms ability to lose an electron. It is important to remember as we stated above that when we talk about the transfer of electrons, we mean the valence electrons. Figure 9 below tells us that the elements in the top right have corner of the periodic table are the most electronegative (ignoring the noble gases due to the octet rule) and the ones in the bottom left are the least electronegative (or the most electropositive).

Key Definitions:

- Electronegativity – the ability of an atom to attract a shared pair of electrons towards itself.



H 2.1																	He ---
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne ---
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.2	S 2.5	Cl 3.0	Ar ---
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr 3.0
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe 2.6
Cs 0.7	Ba 0.9	La-Lu 1.1-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn ---
Fr 0.7	Ra 0.9	Ac-No 1.1-1.7															

Figure 9: A version of the periodic table to show electronegativity. [4]

1.5B: MOVING DOWN THE PERIODS

As we move down the periods (down the periodic table) we know that the elements have more shells. An atom with fewer shells (high up the periods, e.g. Hydrogen) will have its outer shell closer to the nucleus than an atom with a lot of shells (further down the periods), look back at figure 2 to see this pictorially. This, coupled with the inversely proportional relationship between coulomb forces and distances is one factor as to why electronegativity decreases, and atomic radii increases, further down the periods

The other factor to consider is known as ***electron shielding***. Consider things from the nucleus' perspective: you are trying to pull your valence electrons in towards you, so if you only have one shell this is very simple as you will be able to apply a direct force to the valence electrons. But if you have 2 shells, there is now an inner shell that is in your way when trying to pull in the valence electrons and as you move further down the periods there are more and more inner shells in the way. So not only are the valence electrons getting further away from you as we said above, but these inner electrons are effectively shielding your Coulomb force from pulling in the valence electrons. This further explains the trends in electronegativity and atomic radii down the periods.

Example 19: Explain why electronegativity decreases as you move down a period.

Key Definitions:

- Electron shielding – the shielding effect inner electrons have when the nucleus is trying to pull valence electrons towards it.

1.5C: MOVING ALONG THE PERIODS

Previously we have said that all the elements in a period have the same number of shells, therefore the main difference when moving along a period (left to right) is the number of protons and electrons in each element increases (the number of neutrons increases too but this does not affect the properties we are interested in).

Again, we will split the atom into its positive and negative constituents. If we focus on just one period, as you move along the proton number increases, therefore this means there are more protons in the nucleus and the nuclear charge will be increased. If the nuclear charge is larger the further along a period you go, the stronger the Coulomb force is on the valence electrons.

Now since we are looking at the same period the total number of shells is the same, so the electrons are not being shielded any more or less the further down the period. So now we know that for the elements further down a period, the nuclear charge is greater, and the electrons are not being shielded any more than the elements at the start of the period. This means that the Coulomb force between the nucleus and the valence electrons is getting stronger, and hence the valence electrons are being pulled further in by the nucleus. This is what leads to atomic radii decreasing along a period (i.e. the smallest atomic sizes are in the top right corner of the periodic table).

Example 20: Explain how atomic radius changes along a period.

Example 21: On the periodic table, where would you find: the most electronegative element? The element with the largest atomic radius?

Another form of periodicity is ***ionisation energy***, but we will look at this in detail later.

1.6: SUB-SHELL NOTATION

1.6A: REPRESENTATION

Sub-Shell notation is a way of showing the electronic configuration of an element. There is a large integer at the start (which represents the shell), followed by a lowercase letter (representing the sub-shell), followed by an index which tells you how many electrons are in the sub-shell.

For Zinc it looks like $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}$. If we break this down into components it will be easier to understand, we will start by looking at $1s^2$.

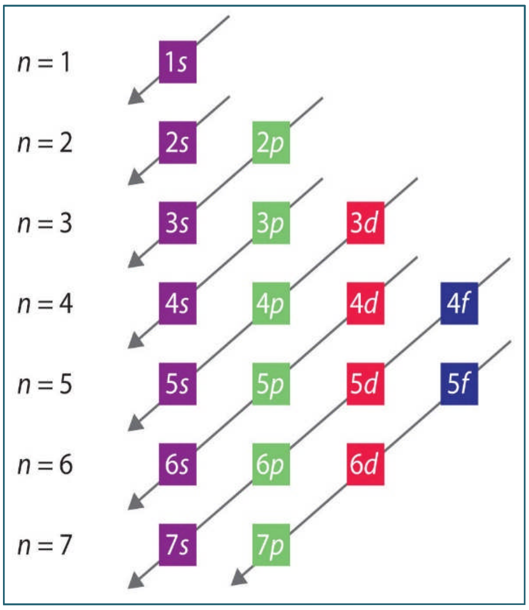
What $1s^2$ means is that we are looking at shell 1, sub-shell s, and it tells us there are 2 electrons there. If it said $1s^1$, that would mean we are still in shell 1, sub-shell s, but there is only 1 electron there (hence, this is the configuration for Hydrogen).

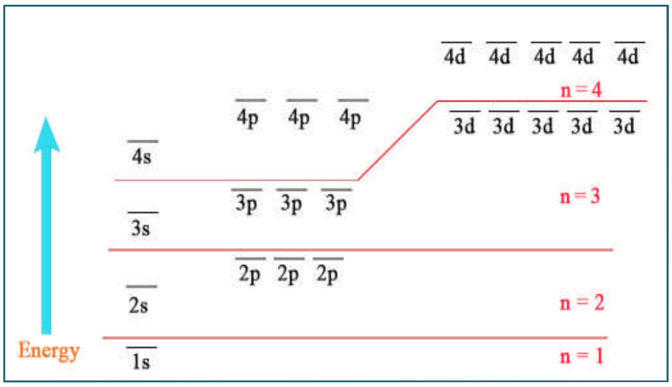
Example 22: Explain what “2p” means, and how many electrons are in $2p^6$?

1.6B: ENERGY LEVELS

The notation is order by energy, i.e. the lowest energy first. As we already know, the larger the principal quantum number, the higher the energy. Therefore, intuitively you would assume the ordering goes 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d, 4f, 5s, … but this is not the case. Above where I told you the configuration for Zinc, you can see that 4s come before 3d. This means we have an exception to the rule. Despite the principal quantum number being larger, overall the 4s sub-shell has less energy than the 3d sub-shell.

There are other exceptions to the rule but you only need to know the sequence up to the 3d sub-shell, beyond that you will be given the ordering.





Figures 10 & 11: Diagrams to show the filling order and the energy of the sub-shells. [5], [6]

Example 23: If 3 atoms have 3, 17 and 19 electrons respectively, what are their sub-shell notations?

There is a shorthand that some people like to use with this notation to save you from writing out the whole thing, where you start off with the noble gas that comes before your element and continue from there. For example, aluminium's configuration is $1s^2\ 2s^2$, $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$, but would be shortened to [Ne] $3s^2\ 3p^1$, because neon is the noble gas that comes before it.

1.6C FILLING SUB-SHELLS

___ **3s (n=3)**

___ ___ ___ **2p (n=2)**

___ **2s (n=2)**

___ **1s (n=1)**

Above is a common example of how one might draw the orbitals in their sub-shells when demonstrating how they fill up, starting from the bottom and moving upwards (in order of increasing energy). For example, when drawn Lithium would look like:

↓ **2s (n=2)**

↓↑ **1s (n=1)**

and Magnesium would look like:

↓↑ **3s (n=3)**

↓↑ ↓↑ ↓↑ **2p (n=2)**

↓↑ **2s (n=2)**

↓↑ **1s (n=1)**

The arrows pointing in opposite directions represent the electrons and their opposing spin values.

Example 24: Draw the configuration of boron.

1.6D: AUFBAU PRINCIPLE

"Aufbau" is the German word for construction, hence the ***aufbau principle*** is followed when filling up orbitals in an atom. It is a general principle and does not always work (for reasons we will not look into), but as far as your Physics degree is concerned you can follow these principles:

1. Begin from the lowest energy levels first. That means the order the sub-shells fill up is 1s 2s 2p 3s 3p 4s 3d etc…
2. Only 2 electrons may fit into a single orbital at a time, one spin-up and one spin-down.
3. When filling orbitals, each orbital must have 1 electron each before you begin to pair them up – this is known as ***Hund's rule***.

Hund's rule is often best visualised, for example let us consider Fluorine. From looking at the periodic table we can see it has 7 electrons, therefore its configuration will be $1s^2\ 2s^2\ 2p^3$. However, if we tried to draw and fill the orbitals as I have shown above, it is not as simple as you may think.

Demonstrated above is the *wrong* way to draw the electrons in the orbitals. If we look back at Hund's Rule we can clearly see we have violated them, as we can see we have paired up two electrons before we have put one in each individual orbital. The correct way would be as follows:

Example 25: Draw the configuration of oxygen.

Key Definitions:

- Aufbau principle – a principle that states that an atom in the ground state will have electrons fill the orbitals from the lowest energy levels first.
- Hund's rule – states that in a sub-shell, each orbital must have at least 1 electron before pairs of electrons can begin to form.

1.7: VALENCE ELECTRONS

The electrons that reside on the outermost shell of an atom are known as ***valence electrons***. E.g. a hydrogen atom has just 1 electron, so it has 1 electron in its outermost shell and therefore has just 1 valence electron.

Example 26: *How many electrons does a Chloride ion with 5 valence electrons have? Write its nuclear symbol.*

Coming back to why the elements in group 13 have only 3 valence electrons and not 13, you can see from figure 7 that the first element in group 13 (Boron, B) has just 5 electrons and so has a $1s^2$ $2s^2$ $2p^1$ configuration, therefore in its outer shell it has just 3 valence electrons.

Element 2 in the group (Aluminium, Al) has a configuration of $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3p^1$, or, as we have learnt the shorthand it is just [Ne] $3s^2$ $3p^1$. Again, here it is easy to see that in the outer shell there are just 3 valence electrons.

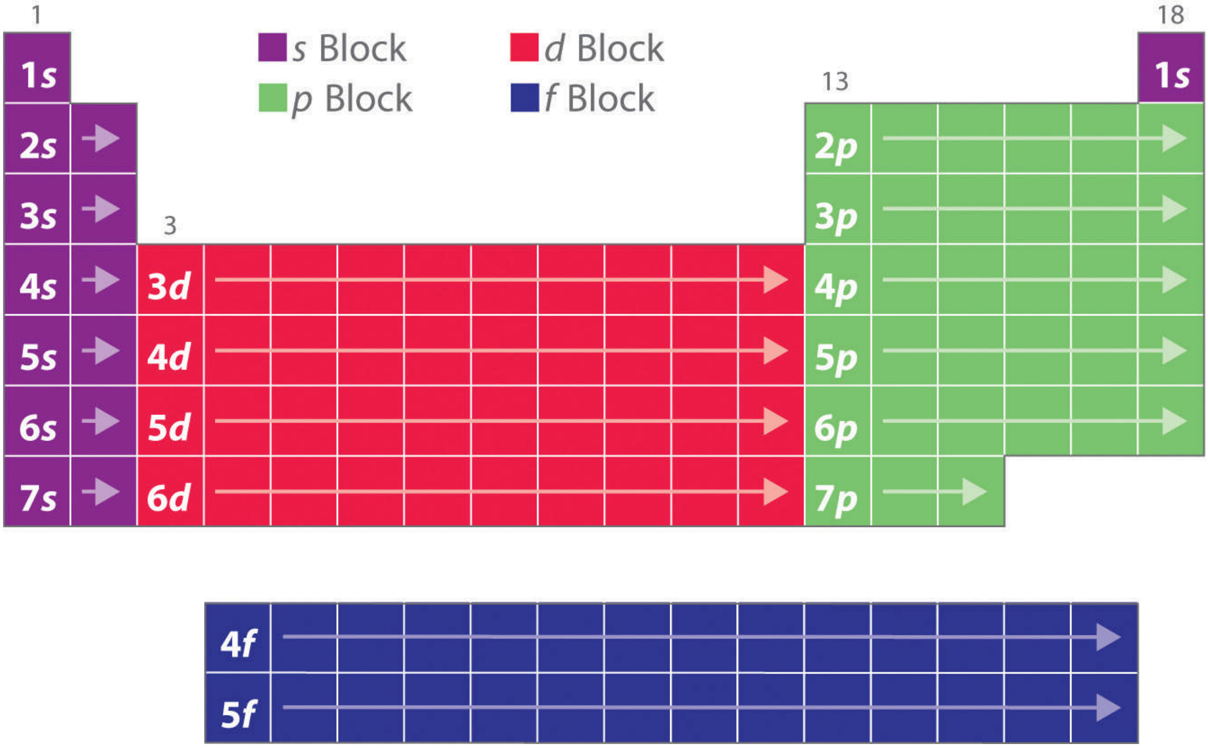
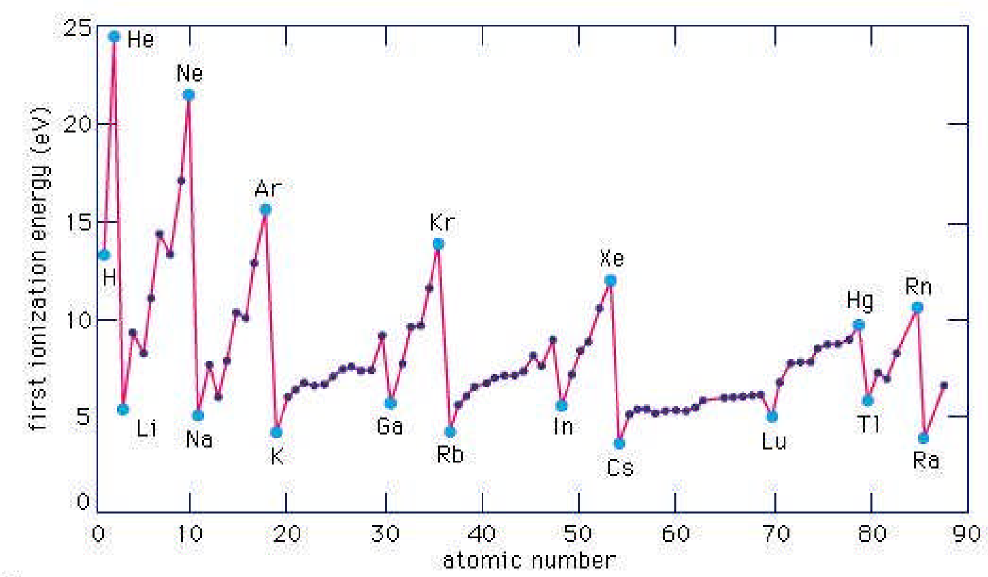


Figure 12: The Periodic Table split into sub-shell blocks. [5]

Now for the third element in group 13 (Gallium, Ga) it gets a bit more complicated as we have a d shell. The electron configuration for Ga is [Ar] $4s^2$ $3d^{10}$ $4p^1$. The definition of valence electron is an electron in the outermost shell, so do not count the 10 electrons in the 3d sub-shell as these cannot be lost in a chemical reaction. Therefore, we just count the electrons in the 4s and 4p sub-shells, giving Gallium 3 valence electrons as predicted. People will often write the electron configuration of Ga as [Ar] $3d^{10}$ $4s^2$ $4p^1$, the reason I did not do this was so that you would not get confused with the ordering of the sub-shells as we have previously said that 3d comes before 4s. In the future, either way is acceptable, but just be sure to remember that 4s *always* fills before 3d.

1.8: IONISATION ENERGY



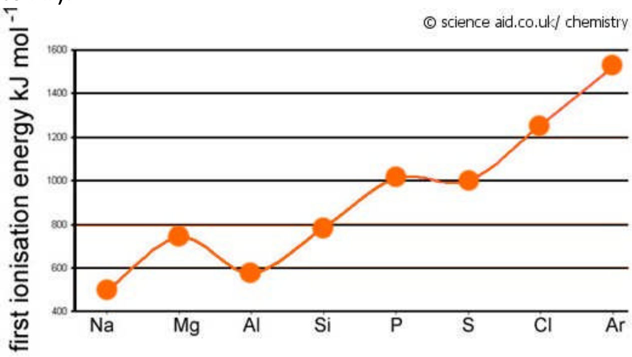
© 2007 Encyclopædia Britannica, Inc.

Figure 13: A graph to show the trend in Ionisation Energy as atomic number increases. [7]

Ionisation energy (which I will refer to as IE) is the energy required to remove a valence electron from an atom or ion. We tend to use the ***first ionisation energy*** as it makes sense to compare the energy required to go from a stable atom to an ion. It is quite closely linked to electronegativity as it is about how to overcome the Coulomb force between the nucleus and its valence electrons.

As you can see the general trend is that as you move across a period the IE increases, and as a new period begins the IE drops drastically. This is because along a period, electronegativity increases, hence more energy is required to pull an electron away. When a new period starts, electronegativity is not as strong, therefore the IE will be lower as the electrons are easier to pull away.

Despite the general increase across a period we can see that there are some slight dips, and this is down to how the electrons fill up their shells and sub-shells. For example, lets looks at the third period (i.e. Na to Ar):



© science aid.co.uk/ chemistry

Figure 14: A diagram to show the ionisation energy across period 3. [8]

We know that Na and Mg both have one and two valence electrons respectively, therefore their valence electrons are in the 3s sub-shell. However, there is a dip as we move from group 2 (Mg) to group 3 (Al). If we compare electron configurations we can see why. Mg = [Ne] $3s^2$, Al = [Ne] $3s^2$ $3p^1$. Aluminium has its valence electron in a 3p sub-shell, and as the 3p sub-shell has a slightly higher energy than the 3s one, this means that on average the valence electron will be found further away from the nucleus. Being further away will mean the Coulomb force will be weaker between the nucleus and valence electron, and there will also be extra shielding from the 3s sub-shell. Both factors mean that this electron is being more weakly held by the nucleus and thus contributing to the decrease in ionisation energy.

There is also a dip in IE as we move from group 5 (P) to group 6 (S), it is only a slight dip but a dip against the trend nonetheless and it is further evidence for the theory of sub-shell structure. P = [Ne] $3s^2$ $3p^3$, S = [Ne] $3s^2$ $3p^4$. The valence electrons remain in the 3p sub-shell, so this is a different scenario to before with Mg and Al, hence the smaller decrease in IE. This is because of the Aufbau Principle, let us look at what the sub-shells look like for Sulphur:

↓↑ ↓ ↓ **3p (n=3)**

↓↑ **3s (n=3)**

[Ne]

As you can see the electron that has been added in last has been added into an orbital where an electron already existed, so we now have a pair of electrons. So, for Phosphorus the electron is being removed from an orbital with just one electron, and for Sulphur the electron is being removed from a pair. The Coulomb repulsion between two negatively charged electrons is enough to make the electron easier to remove from the orbital.

Example 27: Explain why there is a dip in IE when moving from group 2 to group 3 in the periodic table.

Example 28: Explain why there is a dip in IE when moving from group 5 to group 6 in the periodic table.

Key Definitions:

- Ionisation energy – the minimum energy required to remove the most weakly bonded valence electron from an atom or ion.
- First ionisation energy – the minimum energy required to remove the most weakly bonded valence electron from an atom.

2. BONDING

When two or more *atoms* join in a bond a ***molecule*** is formed, when two or more *elements* join they form a ***compound***. So, all compounds are molecules, but not all molecules are compounds. There are many different types of bonding present in compounds and molecules but the main two are *ionic* and *covalent*. In this section we will investigate those two and some of the other types of bonding.

Example 29: If two atoms of the same element joined in a chemical bond, do you have a molecule or a compound?

2.1: IONIC BONDING

Ionic bonding involves the transfer of electrons between elements. Think back to the work we did on ions and remember that it is possible to have positive and negative ions. Ionic bonding is essentials the coming together of equally and oppositely charged ions.

To recap, ions tend to form to suit the octet rule, i.e. group 1 elements have 1 valence electron, so they tend to lose that 1 valence electron to have a full outer shell. This means group 1 elements form 1+ ions. Alternatively, group 7 elements have 7 valence electrons, so they desperately try to gain an extra 1 to fill their outer shell, meaning they form 1- ions.

Combing our knowledge of ions and the fact we know ionic bonding is the coming together of equally and oppositely charged ions, we can predict that group 1 elements will ionically bond with group 7 elements (e.g. Sodium Chloride, NaCl) by the transfer of the group 1's valence electron. Similarly group 2 and group 6 elements can form bonds (e.g. Magnesium Oxide, MgO), but also 2 group 1 elements and a group 6 (e.g. Potassium Oxide, K_2O), etc. We know how an element will react in terms of accepting/losing electrons by looking at their electronegativity.

Example 30: Can sodium ionically bond with oxygen? If so, write whether it is a molecule or a compound and write its chemical formula.

Key Definitions:

- Molecule – two or more atoms joined together in a chemical bond.
- Compound – two or more atoms from different elements joined together in a chemical bond.
- Ionic bonding – a chemical bond formed when two elements exchange electrons to fill their outer shells.

2.1A: DOT-AND-CROSS DIAGRAMS

The most basic and common to represent ionic bonding is through dot-and-cross diagrams, for an example lets look at NaCl:

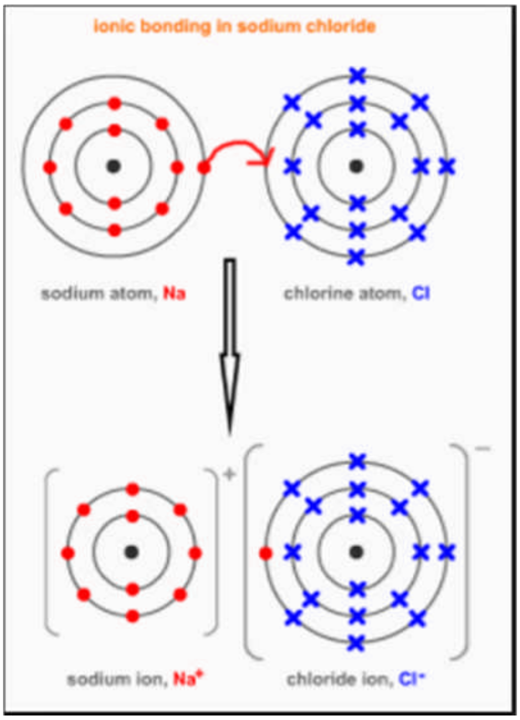


Figure 15: Dot-and-cross diagram for NaCl. [9]

As you can see in figure 15, we are using the basic shell representation shown back in the atomic model section, this depiction is sufficient for showing ionic bonding but sometimes the electron structure is used instead.

The sodium atom's (Na) electrons are represented by red dots, whilst chlorine's atoms (Cl) are represented by blue dots. We know that Na wants to lose its valence electron and Cl wants an extra electron, therefore Na transfers to electron to Cl, forming an ionic bond between the two.

Example 31: Draw a dot-and-cross diagram for magnesium oxide.

2.1B: ELECTRON STRUCTURE REPRESENTATION:

Here there is no new knowledge to learn, just a new way to show what we did above. All we will be doing is showing the electron transfer through the sub-shells as oppose to the dot-and-cross diagram, as this way is more accurate to what we have learnt so far. To make things easy we will stick to using NaCl as the example:

Na: $1s^2\ 2s^2\ 2p^6\ \mathbf{3s^1} \longrightarrow$ Cl: $1s^2\ 2s^2\ 2p^6\ \mathbf{3s^2}\ \mathbf{3p^5}$

⋮

Na^+: $[1s^2\ \mathbf{2s^2}\ \mathbf{2p^6}]^+$ Cl: $[1s^2\ 2s^2\ 2p^6\ \mathbf{3s^2}\ \mathbf{3p^6}]^-$

⋮

$[Na]^+[Cl]^-$

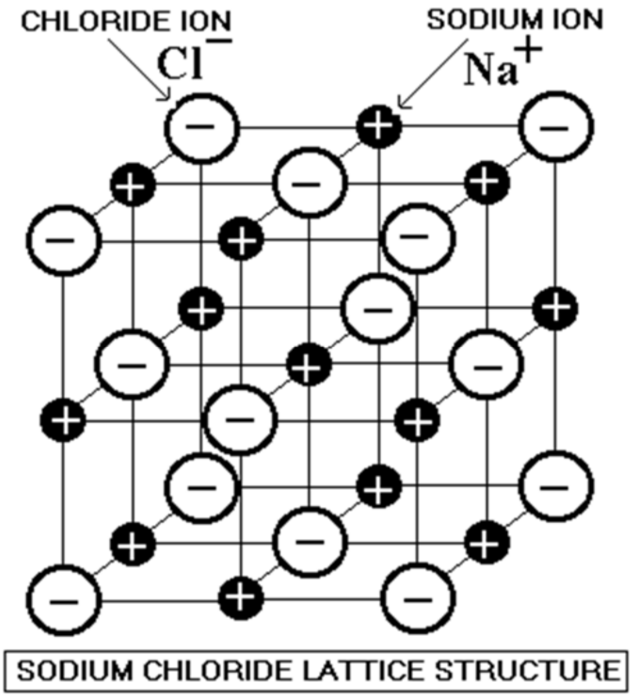
Example 32: Show ionic bonding in MgO through electron structure as shown above.

2.1C: CHARACTERISTICS OF IONIC BONDING

Ionic compounds form a ***giant ionic lattice*** structure which is held together by the Coulomb force of attraction between the oppositely charged ions.

In figure 16 you can see that the alternating ions are held in place by strong ionic bonds (represented by the solid lines). This unit cell will be repeated, giving rise to the "giant" part of the name. This giant lattice is what gives ionic compounds their characteristics:

They have a very high melting point (NaCl is 801°C), meaning that the bond enthalpies must be large as it takes a lot of energy to overcome.



Ionic compounds can conduct electricity, but only whilst molten (liquid) or dissolved. This is because the ions would be free to move around and carry the charge, otherwise the ions are held firmly in place by the ionic bonds.

Figure 16: A diagram of the giant ionic lattice structure of NaCl. [10]

Ionic compounds can be dissolved in water, due to water's polar nature. We will look more into being polar later in more detail, but it just means that part of the molecule is slightly positively charged whilst the other is slightly negatively. These charges mean it is possible for water to pull the ions away from the lattice, hence they dissolve in the water.

Example 33: When can ionic compounds conduct electricity, and why?

Key Definitions:

- Giant ionic lattice – a type of arrangement for elements with an ionic bond, the "lattice" part refers to a regular arrangement whilst the "giant" part means it is repeated over and over with many ions.

2.2: COVALENT BONDING

Where ionic bonding involved the transfer of electrons between elements to fill their outer shells, ***covalent bonding*** involves the sharing of electrons between atoms to fill their outer shell. The atoms can be the same type or different it does not matter.

In contrast to ionic bonding where elements bonded together based off their differences in electronegativity, for covalent bonding it is elements with similar electronegativities that bond together.

Example 34: If two elements had very different electronegativities, would they be more likely to bond ionically or covalently?

Key Definitions:

- Covalent bonding – a chemical bond formed when two atoms share electrons to fill their outer shells.

2.2A: DOT-AND-CROSS REPRESENTATION

We can represent covalent bonding through dot-and-cross diagrams as we did before:

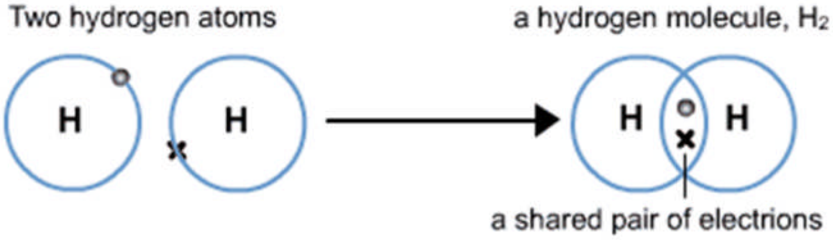


Figure 17: A dot-and-cross diagram to show a hydrogen molecule. [11]

As the two atoms only share 1 pair of electrons, this is a *single* covalent bond. Atoms can share two or three pairs of electrons, making them *double* or *triple* covalent bonds respectively. For example, an Oxygen molecule has a double covalent bond:

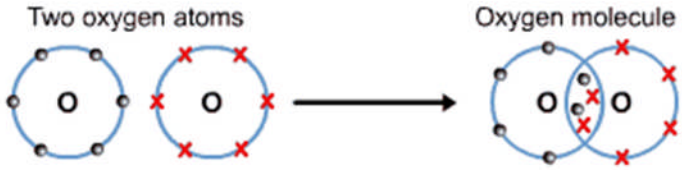


Figure 18: A dot-and-cross diagram to show an Oxygen Molecule. [11]

As you can see in this example they have chosen to only draw the outer shell of the Oxygen atom, this is very common. You are encouraged to do the same when drawing covalent bonds as we are only really interested in the outer shells and it saves time.

Example 35: Draw a dot-and-cross diagram showing the bonding of H_2O.

2.2B: LEWIS STRUCTURES

Another way to represent the bonds is using a single line to represent a single bond, two lines for a double bond, etc. and using a pair of dots surrounding the atomic symbol to represent a ***lone pair***:

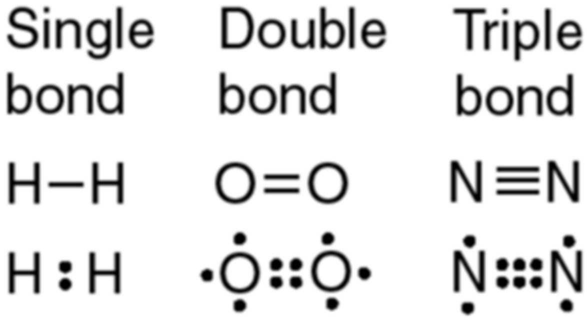


Figure 19: A different representation of covalent bonds. [12]

Example 36: Using Lewis structures, show the bonding of ammonia (NH_3).

Example 37: Using either representation, show the bonding in hydrogen fluoride (HF).

Key Definitions:

- Lone pair - a pair of electrons occupying an orbital in an atom or molecule and not directly involved in bonding.

2.2C: CHARACTERISTICS OF COVALENT BONDNG

Covalent structures can also be giant and are often known as ***macromolecular structures***. Carbon atoms can form these structures in two ways, forming graphite and diamond. The reason Carbon can form these is because it has 4 valence electrons, thus can form 4 strong covalent bonds with itself.

Each structure will have its own set of properties, but the most important thing to note is that covalent bonds can vary from very strong (as strong as ionic in the cases of graphite and diamond) to very weak.

Key Definitions:

- Macromolecular structures – a giant covalent lattice structure, contains many non-metal ions covalently bonded together.

2.3: METALLIC BONDING

In a metal, giant lattice structures are formed. The valence electrons in the metallic atoms disassociate themselves from their atoms and they all come together to form a ***sea of delocalised electrons***. This leaves behind positive metal ions, and naturally there will be an attraction between the positive metal ions and the sea of delocalised electrons. The metallic ions tend to join in their lattice structure, and they become surrounded by the delocalised electrons – this is metallic bonding.

The metallic bonding gives rise to all the typical properties of metal, such as electrical conductivity, the high melting points, etc.

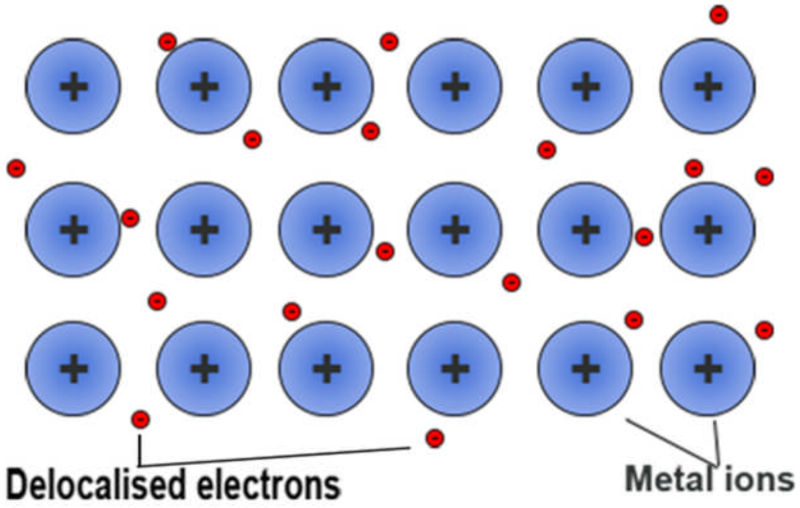


Figure 20: A diagram to show metallic bonding. [13]

Example 38: How many electrons would a potassium atom contribute to the sea of delocalised electrons? What about an aluminium atom?

Key Definitions:

- Sea of delocalised electrons – a metaphorical "sea" that contains electrons that have dissociated themselves from their metal atoms.

2.3A: CHARACTERISTICS OF METALLIC BONDING

Melting/Boiling point: Since the attraction in the bonding of metals is between the positive ions and the delocalised electrons, it makes sense that the more of them that there are, the stronger the bonding in the metal will be. For example, Scandium has 3 valence electrons, so it will form Sc^{3+} ions and contribute 3 valence electrons per ion, this will mean it has a higher melting point than Calcium which only has 2 valence electrons and can only form Ca^{2+} ions. There are other factors that contribute to the melting point of a metal such as lattice structure and ion size, but you do not need to worry about these. Bonding can be weak or strong depending on the material but is generally strong.

Malleable/Ductile: To be malleable is to be shaped easily, and ductile means being draw into a wire. Metals have these characteristics because there is no rigidness to their structure, there are no ions that are held firmly in place and no electrons are fixed where they lie, so they can move around easily.

Conductivity (Thermal and Electrical): Since metallic structures have these delocalised electrons that are free to move around, this means that these electrons can carry kinetic energy (thermal conductivity) or can carry a current as they are charged (electrical conductivity).

Example 39: *Explain the reason for the difference in boiling points of sodium (882.9°C) and magnesium (1091°C).*

2.4: INTERMOLECULAR FORCES

In this section we will be talking about electrons as if they are a ***charge cloud*** as oppose to being in a specific place or shell as we have before, which is a more realistic representation. In these clouds the electrons have a ***probability density*** of where they might be, we use the term probability density because we do not really know where exactly there are as they are always moving.

Key Definitions:

- Charge cloud – a way of considering electron positioning as a "cloud" of probable location.
- Probability density – a way of measuring how probable it is that a random variable (in the example above, electron positioning) is true for that value (i.e. how probable it is that an electron is in that position at any time).

2.4A: POLARISATION

Intermolecular forces (IMF) are weak forces that interact between molecules and one of the reasons they exist is due to ***polarisation of bonds***, in this section we will investigate the polarisation of covalent bonds. The two key bits of knowledge we need we have already looked at: an element's ability to attract electrons towards itself (electronegativity), and the fact that in a covalent bond the electrons are shared between the atoms.

If we had a simple covalent bond with two different elements we know they would be sharing the electrons between them, but if one of these elements is more electronegative than the other, then they will pull the electrons closer towards them – this results in polarisation of the bond. Polarisation of a bond can range from being strongly polarised (a dipole, we will talk about this soon) to being polarised so weakly it makes no difference and can be ignored.

Example 40: *Hydrogen fluoride is a covalently bonded compound, where hydrogen and fluorine have electronegativity of 2.1 and 4.0 respectively – will this covalent bond be polar?*

Key Definitions:

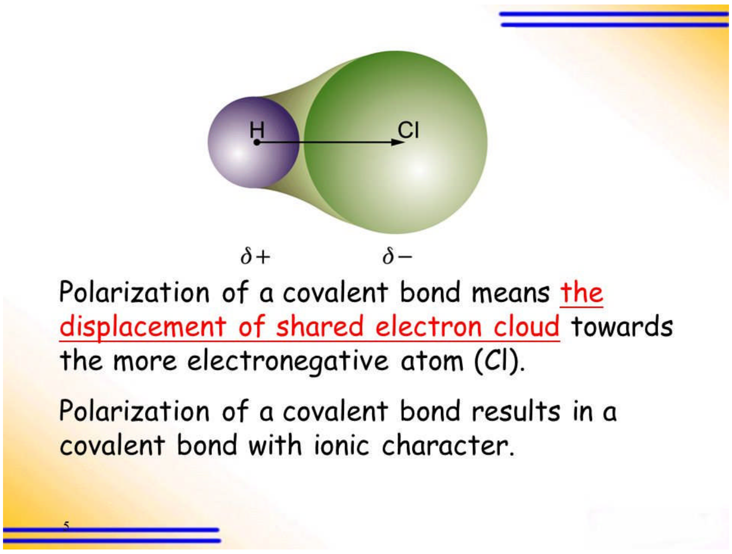
- Intermolecular forces – forces that mediate the interactions between molecules, can be either attractive or repulsive.

- Polarisation of bonds – where there is a separation of the charge in a covalent bond, meaning that one part of the bond is slightly positive and the other part is slightly negative.

2.4B: DIPOLE-DIPOLE FORCES

In a covalent bond, the more electronegative element will be slightly negatively charged, and the other element will be slightly positively charged. This is called a ***dipole***, and the larger the difference in electronegativity between the two atoms, the larger the dipole is. Let us look at HCl as an example:

Figure 21: A picture to demonstrate the polarisation of a covalent bond. [14]



Polarization of a covalent bond means the displacement of shared electron cloud towards the more electronegative atom (Cl).

Polarization of a covalent bond results in a covalent bond with ionic character.

As you can see the spheres represent electron clouds and there is a greater cloud around Cl as it is the more electronegative element in the compound. The "δ" is known as ***delta*** and represents a very small charge.

If two elements had the same or very similar electronegativities (e.g. less than 0.4 on the Pauling scale) then their bonds would be considered ***non-polar bonds***.

If the difference in electronegativities is large enough to create a *permanent dipole* between the two atoms, then the bond is known as a ***polar bond***. However, if the elements have electronegativities that differ by a value larger than 1.7 on the Pauling scale, then they form ionic bonds. Therefore, the range for polar bonding lies between differences in electronegativity of 0.4 to 1.7.

Example 41: *Given the following values for electronegativity, list the following compounds and molecules from least polar to most polar: hydrogen (2.1), chlorine (3.0), oxygen (3.5), fluorine (4.0). The compounds and molecules are: HCl, HF and* O_2.

Key Definitions:

- Dipole – a separation of positive and negative charge.
- Delta – a small, finite change
- Non-polar bond – a covalent bond where there is no dipole
- Polar bond – a covalent bond where there is a dipole

2.4C: VAN DER WAALS FORCES

Van der Waals forces (vdW) are the weakest type of IMF but they exist between all atoms and molecules. Again, we must go back to the idea of electrons existing as charge clouds. The electrons are constantly moving around inside the charge cloud, and at any moment there may be more electrons on one side of the cloud than the other – this is known as a temporary dipole (i.e. for a short amount of time the atom/molecule looks like the example we had above when looking at polarisation).

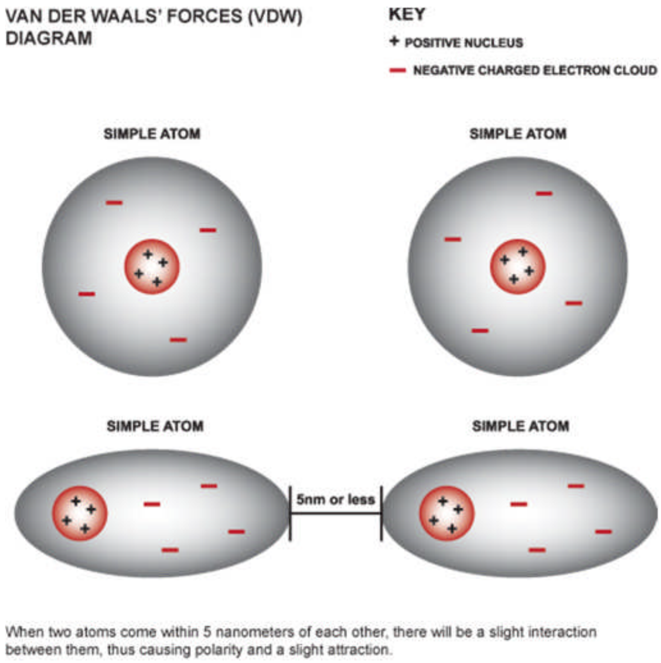


Figure 22: A diagram to show the illustration of how the electron clouds change shape with vdW forces. [15]

Once one temporary dipole has been created, its nature means the small charge on one side of this cloud can induce a temporary dipole in the opposite direction in another electron cloud nearby, and that one can induce another, and so on… Naturally, since these dipoles are in opposite directions then they will be attracted towards each other – if there are a lot of electrons on one side of a cloud, the electrons in a nearby cloud will be repelled by these, leaving a positive charge near the negative charge in the other cloud.

So temporary dipoles have a sort of domino effect, but as these electrons are moving constantly then these temporary dipoles are being created and destroyed all the time. Despite this, they do leave an overall net effect, and that effect is that the atoms are all attracted to one another.

The strength of vdW forces depends on the size of the electron cloud, so larger molecules with larger electron clouds will have stronger vdW forces. This is quite intuitive as the vdW forces depend on the temporary dipoles and the temporary dipoles depend on the electron clouds – the larger the cloud the larger the temporary dipole and the stronger the effect.

The only other important thing to note is that as elements get bigger in atomic size, if their vdW forces are increasing in size then their melting and boiling points will also increase:

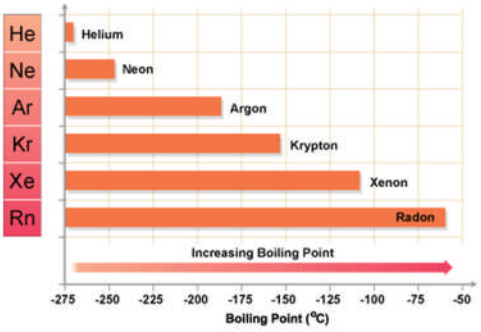


Figure 23: A table to show the boiling points of the noble gases to illustrate the effect of increasing the vdW forces. [16]

Example 42: *Explain how a temporary dipole induces other temporary dipoles in nearby electron clouds.*

Example 43: *Considering the sizes of their atoms, which noble gas out of helium, neon and argon will have the highest boiling point?*

Key Definitions:

- Van der Waals force – a weak type of intermolecular, attractive force between uncharged molecules due to permanent or temporary dipoles.

2.4D: HYDROGEN BONDING

The strongest IMF and the one that occurs under the most specific circumstances, that being you only get hydrogen bonding when you have a hydrogen atom bonded to a highly electronegative element (i.e. fluorine, nitrogen or oxygen). The F, N or O atom draws the bonding electron away from the hydrogen, leaving the hydrogen atom to bond with a lone pair of electrons on another F, N or O atoms from another molecule.

The most common molecules with this type of bonding are ammonia (NH_3), water (H_2O) and hydrogen fluoride (HF). Due to the strength and length of hydrogen bonds, this IMF influences the properties of the substances where it resides. For example, stronger bonding leads to higher boiling points, therefore molecules with hydrogen bonding will have higher boiling points than molecules of a similar nature. E.g. hydrogen fluoride has a higher boiling point than the other hydrogen halides:

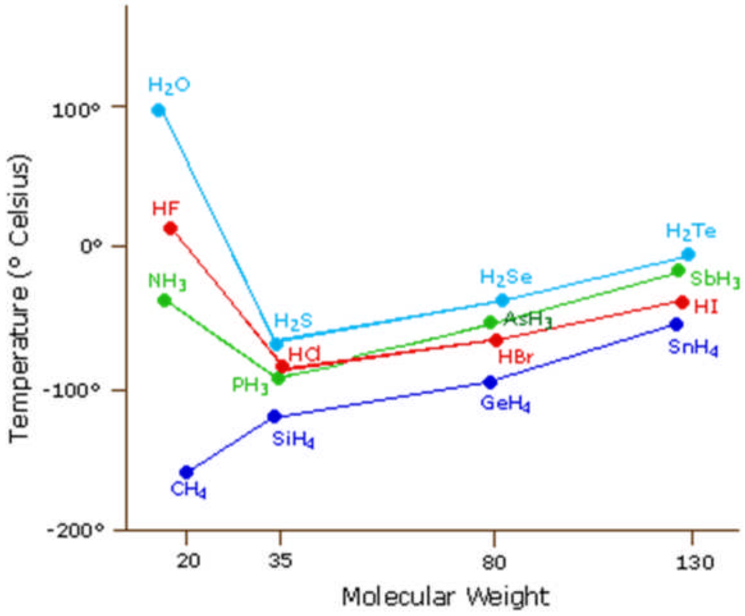


Figure 23: A graph to show the trend in boiling points of the hydrogen halides amongst other molecules to illustrate the effect of hydrogen bonding. [17]

Hydrogen bonds are also the reason why ice is less dense than water. When frozen, H_2O has more hydrogen bonds then when it is a liquid (i.e. ice has more hydrogen bonds than liquid water). As I said above, hydrogen bonds are longer than most, so the H_2O molecules are further apart in ice than in liquid water, hence ice is less dense.

Example 44: *Which type of IMF is stronger, van der Waals or hydrogen bonding?*

Example 45: *Using your knowledge of IMF, which compound out of H_2O and H_2S would have a higher boiling point? (O has electronegativity of 3.5, S has electronegativity of 2.5).*

3. THERMODYNAMICS

3.1: MOLES

An atom is tiny, so small that there is absolutely no way you could see it with the naked eye. When talking about things this small it is hard to get a grasp on how many atoms you have in any given situation. To get around this, scientists found a way to allow us to count how many atoms we have, and this is known as the ***mole/mol, n***.

Key Definitions:

- Mole – the amount of a substance containing the same chemical units as 12 grams of carbon-12.

3.1A: AVOGADRO’S NUMBER

In one mole of a substance there is 6.022140857 $\times 10^{23}$ particles, this number is known as ***Avogadro’s number/constant, N_A***. Avogadro’s number is usually shortened to 6.02 $\times 10^{23}$, and as I said above it corresponds to the number of particles in one mole of a substance.

Example 46: *How many atoms are there on 1 mol of hydrogen?*

Key Definitions:

- Avogadro’s number/constant - the total number of particles in 1 mole.

3.1B: RELATIVE ATOMIC MASS

Before we go into molar mass we need to define what ***relative atomic mass, A_r***, ***relative molecular mass, M_r*** and ***atomic mass, m_a*** are.

Relative atomic mass is sometimes called atomic weight and is not to be confused with atomic mass. A_r is the *average* mass of an atom relative to the mass of 1/12th of carbon-12.

Atomic mass, m_a is defined using carbon 12 and is currently: carbon-12 has an atomic mass of 12 atomic mass units (amu).

M_r is just the sum of all the relative atomic masses (A_r) of all the atoms in the molecule.

In summary, atomic mass is used when talking about a specific isotope, and atomic weight or relative atomic mass, is an average that is used when talking about an element in general. If you had a bag that contained many random carbon atoms, you would say the average weight of carbon in the bag is the relative atomic mass of the carbon, which is usually the number given in the period table (12.011).

Example 47: *What type of mass is given under an element in the periodic table out of relative atomic mass, relative molecular mass and atomic mass?*

Example 48: *What is the relative molecular mass of carbon dioxide (CO_2)?*

Example 49: *What is the atomic mass of:* $^{35}_{17}Cl, ^{197}_{79}Au$, $^{9}_{4}Be$ *and* $^{37}_{17}Cl$?

Key Definitions:

- Relative atomic mass – the average mass of an atom relative to the mass of carbon—12.
- Relative molecular mass – the sum of all the relative atomic masses of all the atoms in a molecule.
- Atomic mass – the specific mass of an individual atom relative to one mass of carbon-12.

3.1C: MOLAR MASS

The mass of one mole of a substance is known as ***molar mass, M***. Molar mass is just the same as relative molecular mass, but it has different units – g mol^{-1} (grams per mole). The units are grams per mole because if you know the molar mass of a substance is for example 70g mol^{-1}, then you know one mole of that substance weighs 70g.

Example 50: *What is the molar mass of: H_2O, NH_3, HBr and MgO?*

Molar mass, mass of substance and the number of moles are all linked, there is a simple calculation which allows you to switch between them all: mass of substance = number of moles x molar mass (i.e. m=n*M).

Example 51: *How much does 3 moles of H_2O, 2 moles of NH_3 and 1 mole of MgO weigh (use your answers from example 50 to help)?*

Below is a table to summarise all the new terms learnt in this section, take your time to go over these and make sure you understand how moles work as this comes up often and people lose marks from making simple mistakes.

	Moles	*Avogadro's Number*	*Relative Atomic/Molecular Mass*	*Atomic Mass*	*Molar Mass*
Symbol	n	N_A	A_r/M_r	m_a	M
Value	N/A	6.02×10^{23}	N/A	N/A	N/A
Units	mol	mol^{-1}	u	u	g/mol

Figure 24: A table to show new terms associated with moles.

Key Definitions:

- Molar mass – the mass of one mole of a substance (the same number as relative molecular mass).

3.2: ENTHALPY

In chemistry, an ***enthalpy change, ΔH*** is described as the exchange in heat energy with the surroundings at constant pressure and is given the units kJ mol^{-1} (kilojoules per mol).

Key Definitions:

- Enthalpy change – the heat energy transferred in a reaction at constant pressure.

3.2A: ENDOTHERMIC AND EXOTHERMIC

An enthalpy change for a reaction can be either positive or negative, and depending on which it is then the reaction will be either endothermic or exothermic.

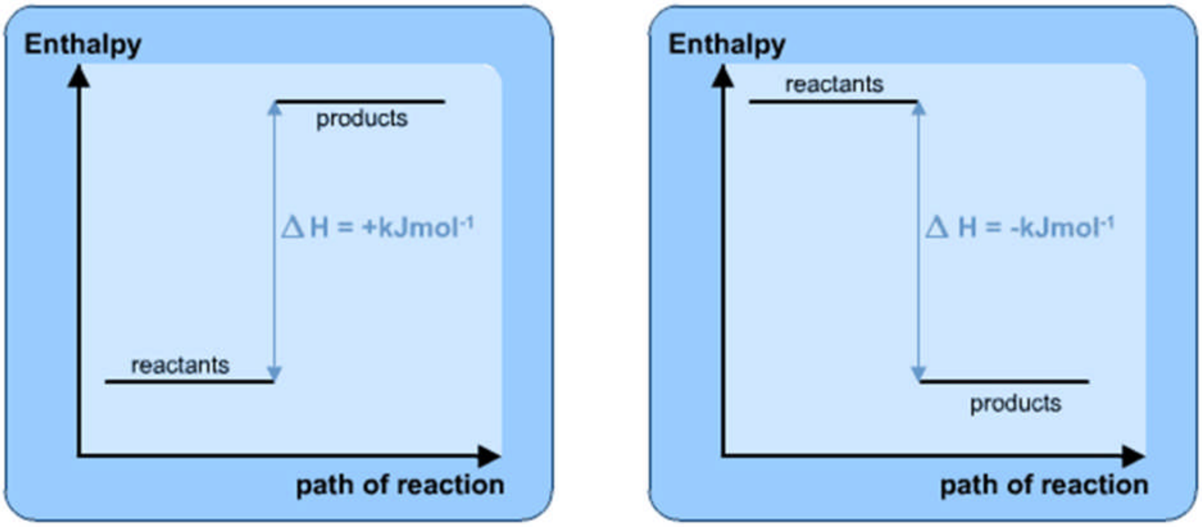


Figure 25: Two graphs to show positive and negative enthalpy change. [18]

On the left of figure 25 is a reaction that shows a *positive enthalpy change*, this means the reaction *absorbs energy* from its surroundings and is ***endothermic***.

On the right the reaction shows a *negative enthalpy change*, meaning the reaction *gives out energy* to the surroundings and is an ***exothermic*** reaction.

Example 52: *If the temperature of the surroundings go from 25°C to 30°C after a reaction, was that reaction exothermic or endothermic? Was the enthalpy change negative or positive?*

Key Definitions:

- Endothermic – a reaction that absorbs energy from its surroundings.
- Exothermic – a reaction that releases energy to its surroundings.

3.2B:MCΔT

MCΔT ("m-cat") is a well known equation that is used to calculate the amount of heat lost or gained in a reaction. The full equation is $Q = mc\Delta T$, where Q = heat lost/gained, m = mass of substance, c = specific heat capacity of substance, and ΔT is the change in temperature of the substance.

Example 53: *Work out Q when 1kg of water is heated from 25°C to 50°C (heat capacity of water is 4181J kg^{--1}).*

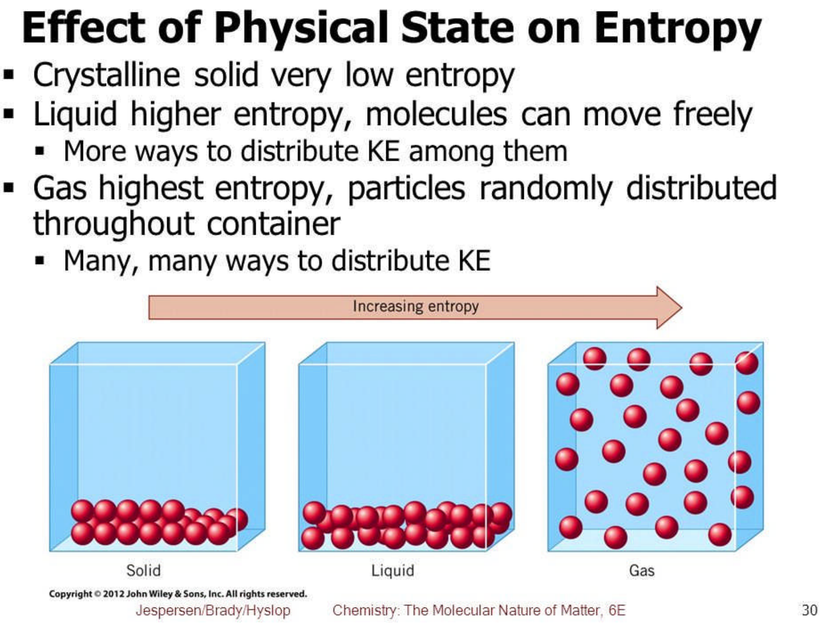
3.2C: HESS'S LAW

Hess's Law is a very simple law regarding enthalpy change, and it states that no matter the route taken, the total enthalpy change of a reaction will always stay the same. I.e. no matter if you go directly from A to B or whether you go from A to C to D to B, the total enthalpy change will still be the same overall.

3.2D: ENTROPY

Put simply, entropy is a measure of disorder. The more ways there are to arrange a set of particles and the more ways there are to share the energy out between the particles, the more disorder and hence the more entropy there is in a system. The second law of thermodynamics states that “the total entropy of an isolated system can never decrease”. Substances love disorder and will always move to try and have a higher entropy.

Entropy is affected by many factors, one of them is the physical state of the substance:



Effect of Physical State on Entropy

- Crystalline solid very low entropy
- Liquid higher entropy, molecules can move freely
  - More ways to distribute KE among them
- Gas highest entropy, particles randomly distributed throughout container
  - Many, many ways to distribute KE

Copyright © 2012 John Wiley & Sons, Inc. All rights reserved.
Jespersen/Brady/Hyslop Chemistry: The Molecular Nature of Matter, 6E 30

Figure 26: A diagram to show how entropy changes with physical state. [19]

Other factors that affect entropy include the number of particles, temperature, and volume – all of these are directly proportional to entropy, i.e. if they increase, so does the entropy.

Example 54: *If system 1 has 7 possible arrangements and system two has 12 possible arrangements, which has a higher entropy?*

Example 55: *What could you do to increase the entropy of a system?*

3.3: KINETICS

3.3A: COLLISION THEORY

As we can see in figure 26 above, in the solid state the particles seem fixed in their position, particles in the liquid state have a little more freedom to move whereas particles in the gas state are a lot more spread out. Particles in gases are always moving, and thus always colliding with each other, but this does not mean that they will react every time they collide. Collision theory dictates the conditions under which particles in a liquid or a gas will collide and react:

1. They must be facing the right direction when they collide.

2. They must collide with at least the minimum amount of kinetic energy to break their chemical bonds (the ***activation energy***).

Example 56: *If two particles in a gas collide facing the right way, does that alone mean they will react?*

The activation energy will change as you go from one reaction to another, and as you would expect reactions with low activation energies happen more readily than ones with a high activation energy. Not all the particles in a gas have the same energy, so if particles in a gas did not have enough energy to react, to give particles more energy to overcome the activation energy you would heat up the whole gas.

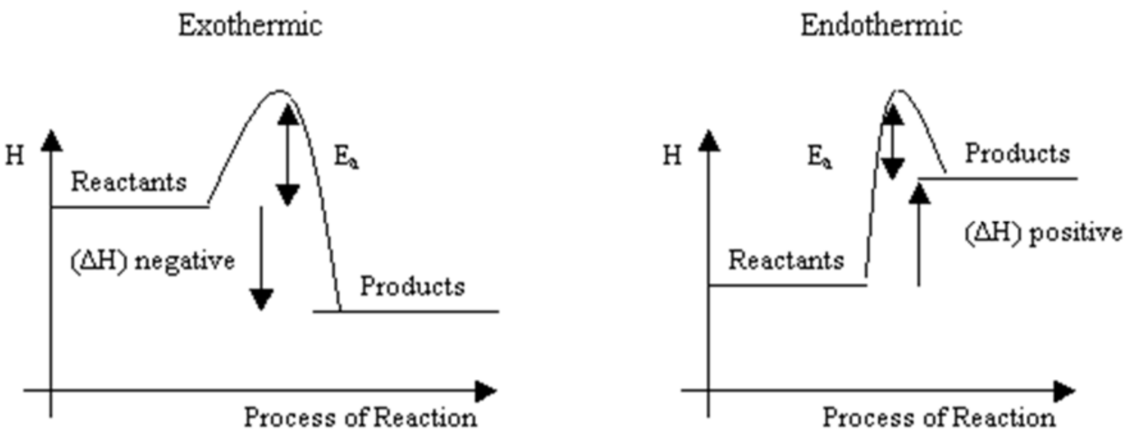


Figure 27: Two graphs to show an enthalpy profile diagram for exothermic and endothermic reactions, where E_a represents the activation energy. [20]

Key Definitions:

- Activation energy – the minimum amount of kinetic energy required for a reaction to start.

3.3B: RATE OF REACTION

Now that we know the conditions required to have a reaction start in the first place, we can investigate what makes these reactions happen faster or slower.

Temperature is one of the main factors of rate of reaction, the higher the temperature the faster the reaction. This is because at a higher temperature all particles have a higher kinetic energy, therefore more of the particles are likely to have an energy above the activation energy, so more reactions occur.

The use of a ***catalyst*** will also affect the rate of reaction – the use of a catalyst increases the rate of reaction. A catalyst offers an alternative reaction pathway which has a lower activation energy than the original, and a catalyst will always remain chemically unchanged at the end of the reaction. Therefore, if the activation energy is lower, more particles will have an energy greater than the activation energy and thus more reactions occur.

Other factors include pressure when using gases, concentration when using liquids and surface area when using solids, where if any of those increase, so does the rate of reaction.

Example 57: Explain how the use of a catalyst affects the rate of reaction.

Example 58: How could you increase the rate of reaction when using a solid?

Key Definitions:

- Catalyst – a substance that increases the rate of a chemical reaction without itself undergoing any permanent chemical change.

3.3C: MAXWELL-BOLTZMANN DISTRIBUTION

As stated above, not all particles in a gas have the same energy. In fact, there is a large range of kinetic energies that these particles could have, and they are shown on a ***Maxwell-Boltzmann distribution***.

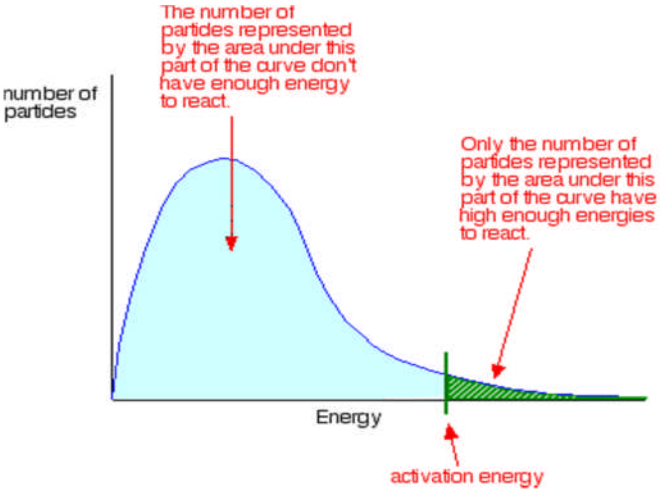


Figure 28: A graph to show the Maxwell-Boltzmann distribution curve for a standard gas. [21]

There are a few important things to note about Maxwell-Boltzmann distribution curves:

- The curve does not start at zero because there are no particles with zero energy.
- Only a small number of particles in the gas have enough energy to take part in reactions.
- The curve never touches the x-axis because there is no maximum energy.
- The area under the curve represents the total number of particles.
- The peak on the curve is the most probable speed.

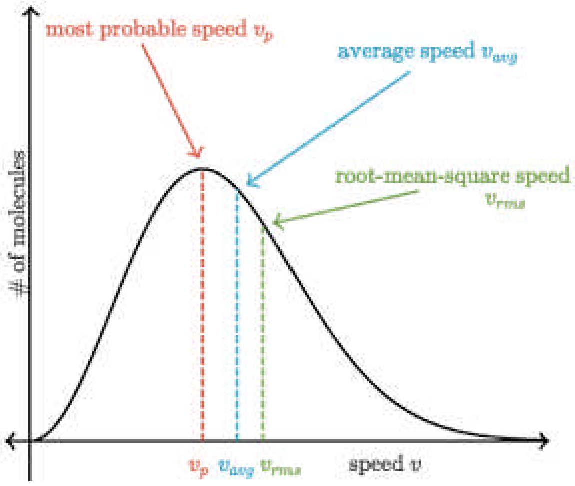


Figure 29: A Maxwell-Boltzmann distribution curve that has been labelled to show points of interest. [22]

You do not need to worry about where the things in figure 29 come from yet, you will learn this during physics 2, but be sure to not confuse the peak of the curve with the average speed.

These distribution curves can be used to show how temperature and catalysts alter the rate of reaction.

Example 59: *What does the highest point on the Maxwell-Boltzmann distribution curve represent?*

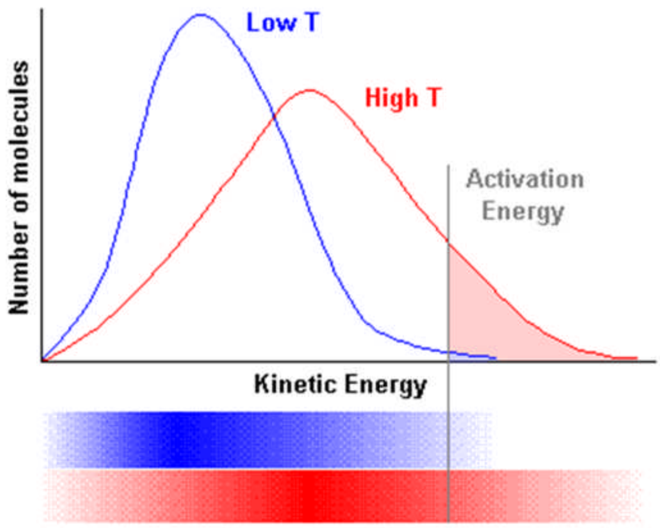


Figure 30: A Maxwell-Boltzmann distribution curve at two different temperatures. [23]

As can be seen in figure 30, changing the temperature alters the shape of the distribution curve. As temperature increases, the most probable speed increases, the number of particles with a higher energy increases whilst the number with a low speed decreases, and there are more particles with a kinetic energy greater than the activation energy. All these things make intuitive sense and agree with everything we said above. However, the most important thing to remember is that the total number of particles has not changed, thus the *area under the curve is still the same*, despite the change in shape.

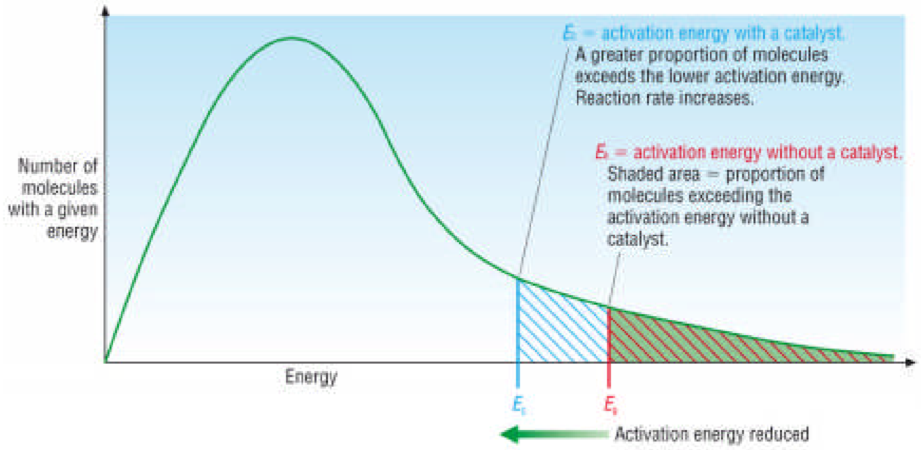


Figure 31: A Maxwell-Boltzmann distribution curve to show the effect of a catalyst. [24]

Again, as we learnt before we know that a catalyst offers an alternative reaction pathway with a lower activation energy, which is exactly what is displayed in figure 31. With a lower activation energy, more particles have a kinetic energy greater than the activation energy, so more particles can react. The shape of the curve does not change at all in this instance.

Temperature and catalysts are not the only things that alter a Maxwell-Boltzmann distribution curve, another factor – molar mass – can affect the shape of a Maxwell-Boltzmann distribution curve:

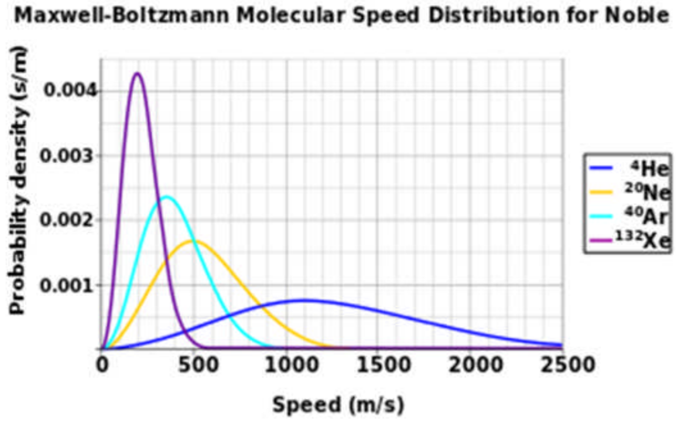


Figure 32: A Maxwell-Boltzmann distribution curve for the noble gases. [25]

As you can see, as the molar mass increases, the most probable speed decreases. This makes intuitive sense, as something gets heavier, it gets slower. Again, for the same number of molecules the area under the graph does not change.

Example 60: How does the increase in temperature affect the shape of a Maxwell-Boltzmann distribution curve.

Example 61: Do the number of particles (the area under the curve) ever change?

Example 62: How would the Maxwell-Boltzmann distribution curve of $^{4}_{2}\boldsymbol{He}$ *compare to* $^{40}_{18}\boldsymbol{Ar}$*?*

Key Definitions:

- Maxwell-Boltzmann distribution – a distribution of the speeds of particles in a gas at a given temperature.

4. EXAMPLE ANSWERS

Example 1 answer: No.

Example 2 answer: Yes, attractive.

Example 3 answer: No.

Example 4 answer: The nuclear strong force overcomes the Coulomb force at short distances.

Example 5 answer: 2 electrons per orbital.

Example 6 answer: Sub-shell f has 7 orbitals so can hold 14 electrons. Sub-shell s has one orbital so can hold 2 electrons. Therefore, f can hold 12 more electrons than s.

Example 7 answer: The electron shell.

Example 8 answer: Electron sub-shell.

Example 9 answer: Orbital quantum number 2 corelates to sub-shell d, which can hold 10 electrons.

Example 10 answer: -3, -2, -1, 0, +1, +2, +3. The range of numbers represents the number of orbitals.

Example 11 answer: Orbital quantum number would be 2, the range of magnetic quantum numbers would be -2, -1, 0, +1, +2.

Example 12 answer: Because there is a further quantum state known as spin, where an electron can either be spin-up or spin-down, hence two unique states inside the same orbital.

Example 13 answer: Na, As, La

Example 14 answer: Yes, yes, no and yes.

Example 15 answer: Yes, it would have a charge of -3: $\boldsymbol{C^{-3}}$.

Example 16 answer: The same number of valence electrons, hence they have similar chemical properties.

Example 17 answer: The noble gases are inert because they already have a closed outer shell.

Example 18 answer: The have the same number of shells.

Example 19 answer: As you move down a period, each element has 1 more shell, meaning their valence electrons will be 1 shell further away, therefore the Coulomb force from the nucleus will be weaker. Also, the extra inner electrons "shield" the valence electrons from the nucleus.

Example 20 answer: In a period the valence electrons of elements are all on the same shell, therefore there is no extra inner electrons to shield the valence electrons from the Coulomb force emanating from the nucleus. As you move along a period, the nuclear charge increases, so the nuclei further along the group will pull the valence electrons in further, ergo atomic radius decreases along a period.

Example 21 answer: The top right (excluding the noble gases) i.e. chlorine and the bottom left corner i.e. francium.

Example 22 answer: We are looking at outer shell 2, sub-shell p, and there are 6 electrons.

Example 23 answer: $1s^2\ 2s^2$, $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$ and $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$.

Example 24 answer:

↓__ ___ ___ **2p (n=2)**

↓↑ **2s (n=2)**

↓↑ **1s (n=1)**

Example 25 answer:

↓↑ ↓__ ↓__ **2p (n=2)**

↓↑ **2s (n=2)**

↓↑ **1s (n=1)**

Example 26 answer: It has 15 electrons, $^{35}_{17}Cl^{+2}$.

Example 27 answer: the most weakly bonded valence electron in group 2 elements is in the s sub-shell, but for group 3 elements it is in the p sub-shell, which has a slightly higher energy. A higher energy means the electron is further away from the nucleus, therefore it is less strongly held by the nucleus and would be easier to pull away, requiring less energy.

Example 28 answer: In both groups 5 and 6, the most weakly bonded valence electrons reside in the p sub-shell, however group 6 electrons are the first to have paired electrons in the p sub-shell, and because there is the repulsive Coulomb force between paired electrons, the valence electron requires less energy to be pulled away from the atom.

Example 29 answer: A molecule.

Example 30 answer: Yes, it would be a compound and its formula would be Na_2O (sodium oxide).

Example 31 answer:

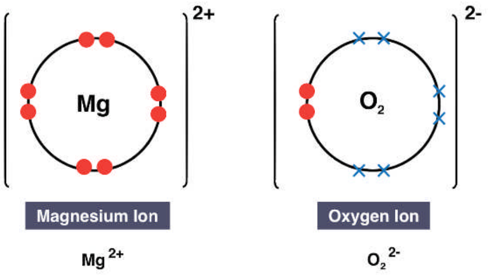


Figure 33: A dot-and-cross diagram for magnesium oxide. [26]

Example 32 answer:

Mg: $1s^2\ 2s^2\ 2p^6\ \mathbf{3s^2}$ → O: $1s^2\ \mathbf{2s^2\ 2p^4}$

⋮

Mg^+: $[1s^2\ \mathbf{2s^2\ 2p^6}]^{+2}$ O: $[1s^2\ \mathbf{2s^2\ 2p^6}]^{-2}$

⋮

$[Mg]^{+2}[O]^{-2}$

Example 33 answer: Ionic compounds can conduct when they are molten/liquid or dissolved in water. This is because when they are solid, their ions are fixed in position and are not free to carry charge, but they are free to carry charge when they are in the afore mentioned states.

Example 34 answer: Ionically.

Example 35 answer:

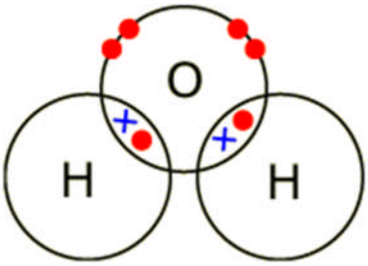


Figure 34: A dot-and-cross diagram showing the covalent bonding of H_2O. [27]

Example 36 answer:

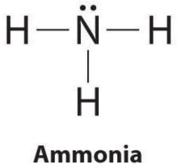
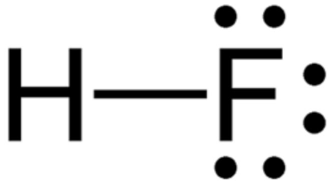
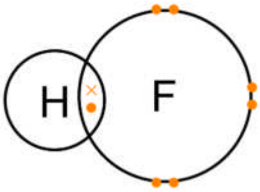


Figure 35: A diagram to show the Lewis structure of ammonia. [28]

Example 37 answer:



Figures 36 & 37: Diagrams to show the bonding in hydrogen fluoride as a Lewis structure and a dot-and-cross diagram. [29], [30]



Example 38 answer: potassium – 1, aluminium – 3.

Example 39 answer: Sodium atoms have 1 valence electron; magnesium atoms have 2. This means sodium atoms will contribute 1 electron to the sea of delocalised electrons and will form 1+ ions, whereas magnesium atoms can contribute 2 electrons and form 2+ ions. There is a stronger Coulomb force of attraction between the magnesium ions and their electrons compared to the sodium ions and their electrons due to the greater difference in charge, therefore magnesium will have a higher boiling point.

Example 40 answer: Yes, fluorine is much more electronegative than hydrogen so it will pull the electrons towards it.

Example 41 answer: (least electronegative) O_2, HCl, HF (most electronegative).

Example 42 answer: A temporary dipole is charge, and like charges repel. Therefore, if there is a slightly negative charge on one side of a cloud due to lots of electrons being there, these electrons will repel nearby electrons to the opposite side of their cloud, creating a temporary dipole in the neighbouring cloud.

Example 43 answer: Argon.

Example 44 answer: Hydrogen bonding.

Example 45 answer: H_2O as the hydrogen bonding will increase the boiling point.

Example 46 answer: 6.02×10^{23}.

Example 47 answer: Relative atomic mass.

Example 48 answer: 44.

Example 49 answer: 35, 197, 9, 37.

Example 50 answer: 18g mol^{-1}, 17g mol^{-1}, 81g mol^{-1}, 40g mol^{-1}.

Example 51 answer: 54g, 34g, 40g.

Example 52 answer: Exothermic, negative.

Example 53 answer: $m = 1kg$, $c = 4181J\ kg^{-1}$, $\Delta T = 25$. Therefore $Q = 1 \times 4181 \times 25 = 104525J$

Example 54 answer: System 2.

Example 55 answer: Increase the number of particles, the volume or the temperature.

Example 56 answer: No, they must also have at least the activation energy.

Example 57 answer: A catalyst lowers the activation energy of a reaction, so more particles will have the minimum energy kinetic energy required for the reaction to occur, and so the rate of reaction increases.

Example 58 answer: You could increase the temperature, use a catalyst or crush the solid to increase the surface area.

Example 59 answer: The most probable speed.

Example 60 answer: The peak of the curve is pushed further forward and slightly lower down than before, and there will be more particles past the activation energy.

Example 61 answer: No.

Example 62 answer: As He is lighter, it would have a higher most probable speed (i.e. the peak of the curve will be further forward), the peak will also be low as there will be a higher % of particles with higher KE so the curve will be spread out over the length of the axis. Ar is heavy, so will have a high peak at the lower KE end of the axis, with not many particles above the activation energy.

5. BIBLIOGRAPHY

[1] - https://en.wikipedia.org/wiki/Bohr_model#/media/File:Atome_bohr_couches_electroniques_KLM.svg

[2] - https://sciencenotes.org/printable-periodic-table/

[3] - http://mshuangchemistry.weebly.com/unit-4-periodicity.html

[4] - http://www.chem.ucla.edu/~harding/IGOC/E/electronegativity.html

[5] - https://saylordotorg.github.io/text_general-chemistry-principles-patterns-and-applications-v1.0/s10-06-building-up-the-periodic-table.html

[6] - https://chemistry.tutorvista.com/inorganic-chemistry/electron-subshells.html

[7] - https://www.britannica.com/science/ionization-energy

[8] - https://chemistry.stackexchange.com/questions/58171/why-does-the-ionization-energy-decrease-anytime-the-atom-size-increases

[9] - https://igcseaid.wordpress.com/notes/coordinated-science-0654/c3-4-ions-and-ionic-bonds/

[10] - https://getrevising.co.uk/revision-cards/giant_ionic_lattice

[11] - https://www.s-cool.co.uk/gcse/chemistry/chemical-bonding/revise-it/covalent-bonding

[12] - http://classnotes.org.in/class11/chemistry/chemical-bonding-molecular-structure/covalent-bond-2/

[13] - https://www.quora.com/What-is-the-nature-of-metallic-bonding

[14] - https://slideplayer.com/slide/4279640/

[15] - https://www.zmescience.com/science/physics/direct-measurement-of-van-der-waals-force-made-for-the-first-time/

[16] - http://www.bbc.co.uk/schools/gcsebitesize/science/edexcel_pre_2011/patterns/groupsrev7.shtml

[17] - https://www.thestudentroom.co.uk/showthread.php?t=1947192

[18] - https://www.s-cool.co.uk/a-level/chemistry/chemical-energetics/revise-it/enthalpy-changes

[19] - https://slideplayer.com/slide/8460786/

[20] - http://www.swotrevision.com/pages/alevel/chemistry/m3_part3.htm

[21] - https://www.chemguide.co.uk/physical/basicrates/introduction.html

[22] - https://www.khanacademy.org/science/physics/thermodynamics/temp-kinetic-theory-ideal-gas-law/a/what-is-the-maxwell-boltzmann-distribution

[23] - http://www.digipac.ca/chemical/mtom/contents/glossary/k.htm

[24] - http://www.chemhume.co.uk/AS%20AQA%20CHEM/Physical/1.5%20%20Kinetics.pdf

[25] - https://en.wikipedia.org/wiki/Maxwell%E2%80%93Boltzmann_distribution

[26] - http://igcse-chemistry-2017.blogspot.com/2017/07/140-draw-dot-and-cross-diagrams-to-show.html

[27] - http://www.bbc.co.uk/schools/gcsebitesize/science/add_aqa/bonding/covalentrev4.shtml

[28] - https://saylordotorg.github.io/text_general-chemistry-principles-patterns-and-applications-v1.0/s12-05-lewis-structures-and-covalent-.html

[29] - https://study.com/academy/lesson/hydrogen-fluoride-uses-formula-quiz.html

[30] - https://commons.wikimedia.org/wiki/File:Hydrogen-fluoride-2D-dot-cross.png