As Level Chemistry OCR A 2015

Benjamin Chalmers

April 2, 2016

This is a series of rough notes for the new spec examinations in Chemistry. They will not be whole and I will be skimming over areas of the course that I know well.

I will be writing this using the specification as my guide. H032 is the course and you can find the original document through Google. This document will be continuously referencing this spec so if you are wondering what all the references are too.

Contents

Module 1

Practical Skills in Chemistry

Practical skills are crucial to chemistry. Chemistry is a practical subject; as such we should understand how to correctly carry out our experiments. Practical skills are a recurring theme throughout the other 4 modules so a good knowledge of these skills is vital to success.

1.1 The doing 1.1.1 & 1.1.2

Planning is a crucial to any and all experiment doing. In this course you should be able to do several things with ease.

Firstly you should understand the range of equipment available and there appropriate usage. You should then have the mental capacity to apply this knowledge to a given situation and, in so doing, design a practical. This understanding comes with time and I will not go into much detail.

Secondly you should understand these distinctions. *Independent* variables are ones which the experimenter changes e.g. the temperature of the heater. *Dependent* variables depend on the independent ones and are measured e.g. the amount of gas released from the reaction. *Control* variables are ones which remain constant and are controlled by the experimenter e.g. the amount of substance added.

Because I like maths think of it like this. Let y be the dependent, x be the independent and c be the control/constant:

$$y = f(x) + c$$

By keeping c constant and changing x we can derive $f(x)$ which is what many experiments try to do. Determining the relationship between the independent and the dependent variable.

Lastly you should be able to evaluate the experimental method to determine whether or not it is appropriate to find the expected outcomes. This part requires critical thinking and an understanding of modules 3-4

Implementing   is more about usage. I will not go into it fully here but here is an overview.

You need to know your units, techniques and how to use the apparatus. Ask your teacher to show you the techniques and how to use the apparatus. The units will be visited as we explore the rest of this spec.

1.2   The reviewing 1.1.3 & 1.1.4

Reviewing   is necessary, it comprises two parts, that of analysis and of evaluation.

Analysis   simply the processing and interpretation of qualitative[1] data combined with an understanding of the maths skills involved to explore quantitative[2] data. Basic statistics skills required are as follows:

$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} \tag{1.1}$$

Technically not necessary but makes your PAGs feel more exact:

$$y = a + bx \quad b = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2} \quad a = \bar{y} - b\bar{x} \tag{1.2}$$

Plotting graphs is important because this exam uses mostly graphical methods to find things such as gradients (which, at a point, it the gradient of the tangent to the curve often expressed as $\frac{dy}{dx}$). Just remember to use a good scale when drawing them.

Evaluation   is the process in which we look back at the plan and the method and, well, evaluate it. You need to understand the limits of the procedure used, identifying anomalies and refine the experimental design by suggesting improvements to the procedures and apprentice.

---

[1]Observed data e.g. colour and effervescence
[2]Data that is measured with a numeric output e.g. temperature

Module 2

Foundations in Chemistry

This part is all about understanding the basics. If you took triple science like me you should know the vast majority of this module.

2.1 Fundamentals in chemical semantics 2.1.1

Isotopes are atoms of the same element with different atomic masses.

Atomic Structure is, in this section, in reference to the number of protons neutrons and electrons found in an atom. Understanding that the Relative atomic mass of a proton is ≈ 1 a neutron ≈ 1 and an electron is negligible. OCR like questions which involve giving the repetitive isotopic mass of an element and ask you to calculate the number of neutrons o/e.

Mass spectrometry is a tool chemists use to identify the relative mass of ions. You need to be able to look at the readout from a mass spectrometer.

First let us examine how a mass spectrometer works (you will see more of this). Fist we put a sample of the substance we are testing in the machine. The sample is vaporized and ionized to form positive ions. These positive ions are then accelerated and separate based upon the weight of the ion. The readout will give the mass-to-charge ratio on the x axis and relative abundance on the y. (there is a diagram in your book if I don't get round to making one.) The peaks represent isotopes if the substance is an element.

In this section we use the percentage abundance[1] to work out a mean atomic mass.

Relative atomic mass is a term I have been using which has so far been left unexplained. I will clarify its meaning now. Relative atomic mass is the mass of an atom relative to $\frac{1}{12}$ the mass of ^{12}C. This term is almost identical to

---

[1] Derived from relative abundance

the terms relative isotopic mass, relative molecular mass and relative formula mass. Mr is generally the algebraic identifier used and is the molar mass of a substance (which is in $g\,mol^{-1}$). In these notes if I say Mr_{NaOH} I am referring to the Mr of Sodium Hydroxide.

In case you have not managed guess it, to work out the relative formula mass one simply summates the atomic masses of the elements in the formula. The subscripts in formula mean x of this e.g. there are two chlorine atoms in C_2.

2.2   Basics in ionic compounds and equations 2.1.2

Shells   are a concept that, for now, you just need to accept. We will explore it further soon but just accept it for now. They contain electrons and want to be full. An atom with unfilled outer shell may loose an electron, or gain an electron from another atom. When this happens we call them ions.

The amount of electrons that an atom will loose/gain is fairly predictable. Looking only at the first three periods on the periodic table, the group numbers refer to the number of electrons the atom has in the unfilled outer shell. Group 0 has a full outer shell, group 7 has 7 electron in the outer shell, group 6 has 6 etc.

Now given that there are a maximum of 8 electrons in the outer shell, and an atom wants to be stable, an element in group 7 is going to do the efficient thing and gain an electron, whilst an atom in group 1 is going to loose one. So take, for example Lithium and Chlorine. Lithium is in group one and will loose an electron. Chlorine is in group 7 so will gain an electron. If lithium gives an electron to chlorine it becomes Li^+ and chlorine becomes Cl^-. Opposite charges attract and so we form an electrostatic bond between Lithium and Chlorine. We call this substance Lithium Chloride and this bonding mechanism is called *Ionic Bonding*. To succinctly define ionic bonding would be as follows:

> Ionic bonding is a bond formed by the electrostatic attraction between two oppositely charged ions.

Ions   are atoms or compounds with a charge. There are some ions you need to remember, and remember there suffix too as it will help you name them. NO_3^- is the -nitrate ion, CO_3^{2-} is the -carbonate ion, SO_4^{2-} is the -sulfate ion, OH^- is the -hydroxide ion, NH_4^+ is the amonium- ion, Zn^{2+} is the zinc- ion and Ag^+ is the silver- ion. The reason for all the - is that it makes creating the words easier. For example, silver nitrate is $AgNO_3$. The Positive ion then the negative one.

Hint If the word has the suffix -ate, it means that oxygen is present in the ion

Equations   in chemistry refer to a system of expressing a chemical reaction. For example: $2\,NaOH + H_2SO_4 \longrightarrow Na_2SO_4 + 2\,H_2O$. As you can see we have

the reactants on the right, products on the left and the big numbers balance the equation acting as the molar ratios for stoichiometry.

2.3 The mole

Moles are a new way to look at measuring quantity. Instead of looking at how much of a substance we have by weighing it we can look at how much we have of a substance by looking at the number of particles we have of it. 1 mole is equal to 6.02×10^{23} particles. This is all, usefully, designed around the gram. To show you what I mean take our good friend ^{12}C. If I get 1 mol of ^{12}C I will have 12 grams of it. This relationship works by design. So now we have the formula $m = nM_r$ where $n =$ number of moles and $m =$ mass.

Concentration is a simple extension. Simply take the number of moles dissolved in a given volume of solvent then divide it by the volume. Concentration is measure it in mol dm^{-3}.

A mole of gas fills, in standard conditions (RTP), 24.0 dm^3 of space. The number of moles is directly proportional to the space filled. You can find this information on the formula sheet under "Molar gas volume".

When the substance isn't under standard conditions the ideal gas equation is used, $pV = nRT$. Lucky this is also sort of given. They give us a number called the "Gas constant". This number gives us the units (J mol^{-1} dm^{-3}). We know that pressure is measured in pascals, which have the S.I. unit N m^{-2} and volume has the S.I. unit of m^2. So the product of volume and pressure is to be N m which is, as we all know, J. Using this mental gymnastics we can express the units like so, Pa m^3 mol^{-1} K^{-1}. and we know this to be equal to 8.314. So the given (but hidden) formula is,

$$8.314 = \frac{pV}{nT} \tag{2.1}$$

The Units used in this calculation have no given conversions, The exam may well give T in degrees centigrade and p in atm. Here are some conversions:

1 atm = 101 KPa (3 S.F)

0 C = 273 K (3 S.F)

Empirical formula is the simplest whole number ratio of atoms of each element present in a compound.

Molecular formula the number and type of atoms of each element in a molecule.

Determining formula   is a necessary part of this exam. They love questions along the lines of "Raheem has found that his substance has a composition by mass of 70.00% C, 6.67% H and 53.33% O. (a) work out the *empirical formula* (b) given the Mr of the compound is 180, work out the *molecular formula*."

How is this to be approached? Well we have been given the %age composition by mass. If we assume the %age mass to be actual mass (given that we are working out a ratio) we can convert into moles.

$$Mr_\text{C} = 12.0$$

$$Mr_\text{H} = 1.0$$

$$Mr_\text{O} = 16.0$$

$$\text{Molar ratio (C:H:O)} = \frac{70.00}{12.0} : \frac{6.67}{1} : \frac{53.33}{16.0}$$

$$\text{Molar ratio (C:H:O)} = 3.33 : 6.67 : 3.33$$
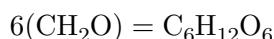
$$3.33 : 6.67 : 3.33 = 1 : 2 : 1$$

Now we have an answer to part (a). CH_2O. To work out part (b) we need to set up an equation:

$$n \times Mr_{\text{CH}_2\text{O}} = 180$$

$$Mr_{\text{CH}_2\text{O}} = 30.0$$

$$n = \frac{180}{30.0}$$

$$n = 6$$

$$6(\text{CH}_2\text{O}) = \text{C}_6\text{H}_{12}\text{O}_6$$

Hydrated salts   are calculated in much the same way. They are expressed like this $CuSO_4 \cdot nH_2O$ and you will be given some numbers to workout n. Heating a substance removes the H2O making it anhydrous. To Hydrate simply devolve the salt in water and evaporate the water very slowly.

Atom economy and %age yield   are as simple as they sound. %age yield is in reference to the percentage of the theoretical yield that was actually yielded. Atom economy simply refers to the number of waisted atoms (atoms that form waist products). Simply apply logic and understand these two concepts in terms of industry.

2.4 Acids 2.1.4

**The acids to remember** are the following:

- HCl is Hydrogen Chloride

- H_2SO_4 is Hydrogen Sulphate

- NOH_3 is Nitric Acid

- KOH is Potassium Hydroxide

- CH_3COOH is Ethanoic Acid (although it is commonly called Acetic Acid).

Acids release H^+ ions when in aqueous solution. To examine the strength of an acid we must look at the dissociation of the H^+ ions. Take for example HCl. The dissociation of HCl in aqueous solution looks like this,

$$HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$$

As you can see all of the hydrogen atoms have dissociated. This would make HCl a *strong acid*.

Where the H^+ ions only partially dissociate we call it a *week acid*. Take Ethanoic acid, its dissociation in aqueous solution looks like this,

$$CH_3COOH(aq) \rightleftharpoons H^+(aq)CH_3OO^-(aq)$$
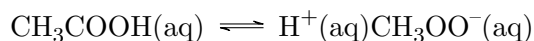
As we can see the H^+ ions haven't entirely dissociated. The $\rightleftharpoons$ implies that the reaction is incomplete and forms an equilibrium, So the acid hasn't completely dissociated.

There is a point to be made that not all ionic compounds with hydrogen atoms are acids. It is only those compounds that form H^+ ions when dissolved in aqueous solution that we call acids.

The common bases are metal oxides, metal hydroxides, metal carbonates and ammonia, NH_4. Bases neutralise an acid and form a salt.

An Alkali is a special type of base which, when dissolved in water, releases hydroxide ions. For example take the base $Mg(OH)_2$,

$$Mg(OH)_2(s) + aq \longrightarrow Mg^{2+}(aq) + 2\,OH-(aq)$$
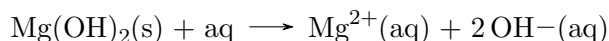
We can see that $Mg(OH)_2$ is an alkali as it releases OH^- ions when dissolved in aqueous solution.

The alkali to remember   are the following:

- NaOH is Sodium Hydroxide

- KOH is Potassium Hydroxide

- NH_3 is Ammonia

However you will be expected to know how to peace together bits you already know to construct your baces/alkali formula.

You need to remember   that $H^+ + OH^- \longrightarrow H_2O$, $CO_3^{2-} + 2\,H^+ \longrightarrow H_2O + CO_2$ and finally $O^{2-} + 2\,H^+ \longrightarrow H_2O$. Using these ionic equations you should be able to form full equations.

Titrations   are a piratical technique to achieve a neutralisation reaction. We take an acid and a alkali and we slowly add one to the other using a burette. This is a PAG and you probably will have done this.

The preparation of a standard solution simply involves dissolving a exact and known mass of ionic compound and dissolving it in a know volume of water. This is done in a volumetric flask.

2.5   Redox 2.1.5

OIL RIG   is a fantastic acronym. Oxidation Is Loss, Reduction is gain. Remembering this is vital. If we describe a reaction as having *oxidised* X, we mean to say that X has lost electrons. If a reaction is described as having *reduced* X, we mean to say that X has gained electrons.

To write a redox reaction we have equations like this:

$$\overset{\text{OX: } -2e^-}{\overbrace{2\overset{0}{\text{Na}} + \underset{\text{RED: } +2e^-}{\underbrace{\overset{0}{\text{Cl}_2} \longrightarrow 2\overset{\text{I}}{\text{Na}}^+ + 2\overset{-\text{I}}{\text{Cl}}^-}}}}$$

We use Roman numerals to indicate oxidation numbers, memorise the following oxidation numbers:
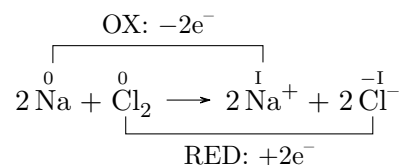
- Oxygen has the oxidation number -2 unless in peroxide, in which case it is -1

- Hydrogen has the oxidation number +1 unless in a metal hydride in which case it is -1

- Fluorine has the oxidation number -1

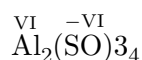So to work out whether a chemical has been oxidised or reduced we do the following.

1. Find the balanced symbol equation,

   $$2\,Al + 3\,H_2SO_4 \longrightarrow Al_2(SO_4)_3 + 6\,H_2$$
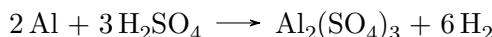
2. Then we fill in the oxidation numbers for the ones we know,

   $$2\,\overset{0}{Al} + 3\,\overset{II}{H_2}\overset{-II}{SO_4} \longrightarrow Al_2(\overset{-VI}{SO_4})_3 + 6\,\overset{0}{H_2}$$
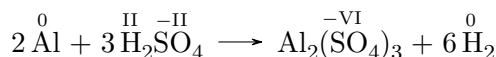
3. The $Al_2(\overset{-VI}{SO})3_4$ has no overall charge so the oxidation numbers must add to 0,

   $$\overset{VI}{Al_2}(\overset{-VI}{SO})3_4$$

4. Now we have $\overset{VI}{Al_2}$ we can see that $\overset{III}{Al}$. So Aluminium went from Al to $\overset{III}{Al}$ meaning it has been oxidised in this reaction.

5. The hydrogen went from $\overset{II}{H_2}$ to H_2. This is a reduction so we say hydrogen has been reduced.

A faster way to instantly know is to look at the oxygen. We can see that Hydrogen has lost oxygen in this reaction while Aluminium has gained oxygen. By looking at it this way we can very quickly see what has been reduced and what has been oxidised.

In summary oxidation numbers refer to the number of electrons individual atoms in compounds have lost/gained. They are like charge but apply to atoms and not the overall compound. They are used to explain whether a reaction has oxidised an atom or reduced it.

2.6 Electron structure 2.2.1

Shells are areas where there is a heigh probability of finding an electron. They are split by looking at major energy levels. The period an atom is in indicates how many shells it has. The number of electrons that can fit into a shell can be worked out by $2n^2$ where n is the shell number.

**Shells are sub-divided** into sub-shells. The ones you need to know are as follows,

- s orbital which can hold 2 electrons, one in all shells

- p orbital which can hold 6 electrons, one in all but shell 1

- d orbital which can hold 10 electrons, one in all but shells 1 & 2

They fill in order.

Orbitals   are regions around the nucleus which can hold up to two electrons, both have opposite spin. This diagram is of a P orbital and the arrows indicate the spin,

$$
\begin{array}{ccc}
\text{x} & \text{y} & \text{z} \\
\downarrow\uparrow & \downarrow\uparrow & \downarrow\uparrow
\end{array}
$$
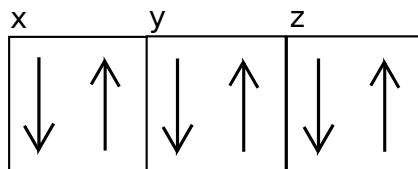
This is a Full P orbital and as you can see, each sub-orbital (denoted by the box) contains two electrons of opposite spin. They don't, however, fill sequentially. It take less energy to fill like this,

$$
\begin{array}{ccc}
\text{x} & \text{y} & \text{z} \\
\downarrow\uparrow & \downarrow & \downarrow
\end{array}
$$
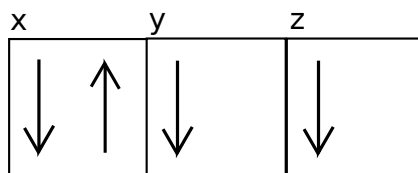
X get the first, Y gets the second Z gets the third and X gets the last. All the orbitals work in a similar way and the number of sub-orbitals can be found by dividing the maximum electron capacity by 2.

Order of fill   is as follows, $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$ in the standard format $x\text{s}^n$ where x is the shell and n is the number of electrons in the shell.

   The examination may well ask you to write the electron configuration of an atom. Unless otherwise instructed, a short cut is to use a noble gas as a base. For example if I said write the electron configuration of sodium you can say $[\text{Ne}]3\text{s}^1$. You need to know how to do this for all elements upto and including Kr

Energy levels   are the reason different shells fill differently. As we go up the shells we also ascend in energy level. The most interesting part is the 4s sub-shell and the 3d sub-shell. The 4s sub-shell and the 3s sub-shell have very similar energy levels. The 4s sub-shell is, however, slightly lower so the 4s fills first. When the 3d sub-shell fills the energy level falls meaning, the 4s fills before 3d and the 4s empties before 3d. This is important when looking at the electron configuration of D Block ions.

2.7   Bonding 2.2.2

Ionic bonding   is the first of the two types of bonding I need to cover. As mentioned before,

Ionic bonding is a bond formed by the electrostatic attraction between two oppositely charged ions.

We have cations, which are positively charged ions, and anions, which are negativity charged ions. When the cation and the anion meet they form a ionic bond. It is, as you guessed, the bonding which holds together ionic compounds like NaCl.

Dot-and-cross diagrams are the same as they have always been. Used for drawing the simplest of ionic bonds, that of metal - non-metal. Just remember the square brackets, the outer shell is drawn and the charge goes at the top right of the brackets. (potential for diagram if I have time)

Giant ionic lattices are the result of ionic bonding. This is what gives ionic compounds their crystalline structure. Take sodium chloride, each Na^+ ion is surrounded by 6 Cl^- ions and vis-versa, they are strongly attracted in all directions. This gives it a cubic structure and is why table salt breaks into small cubes.

Ionic bonds physical properties are fairly obvious. The strong electrostatic forces within a giant ionic lattice require high energy to break. This makes ionic compounds almost always *solid* at room temperature and mean that they have a *high* boiling point.

Ionic compounds will usually dissolve in polar solvents, such as water. The polar molecules in the solvent break down the lattice creating dissociated ions, which are then surrounded by the solvent. However some ionic compounds will not be very soluble. This is because the electrostatic attraction between the ions may be too strong for a polar solvent, such as water, to break down. In general the greater the ionic charge, the less soluble the ionic compound will be.

Electrical conductivity in a solid ionic compound is zero. This is because the ions are not free to move around. However if the compound is dissolved or melted it will be able to conduct electricity. This is because the ionic bonds have been broken down and the ions are free to carry charge (mobile charge carriers).

- Have heigh melting and boiling points

- Tend to dissolve in polar solvents

- Only conduct electricity when in liquid state or dissolved in aqueous solution.

Covalent bonding   , to quote the specification, is "the strong electrostatic attraction between a shared pair of electrons and the nuclei of the bonded atoms."

- Non-metallic elements such as H_2 and O_2 form covalent bonds.

- Non-metallic compounds such as H_2C and CO_2 form covalent bonds.

- Even polyatomic ions are covalently bonded such as NH_4^+

Dot and Cross   diagrams are very similar to the dot and cross diagrams for ionic bonding. Instead of drawing them septate in there own square brackets we simply draw them as overlapping circles with dots and crosses for the various electrons.

There are the following three types of covalent bonding that you are expected to know about,

1. Single covalent bonding, this is where there is one shared pair of electrons per nuclei.

2. Multiple covalent bonding, this is where there are multiple pairs of shared electrons per nuclei

3. Dative covalent bonding, this is where the shared pair is supplied by only one of the atoms.

You will be expected to draw dot-and-cross diagrams with atoms of up to six electron pairs, including lone pairs. This means the bonding seen in SF_6 will roughly be the most complicated.

NH_4^+ is a good example of a dative covalent bond. A H^+ ion meets amonia and amonia provides the electron pair for the covalent bond.

Average Bond Enthalpy   is simply a measure of the average amount of energy required to break say a $Br-Br$ bond. This acts as an indicator to the bonds strengthen, the larger the value of the average bond enthalpy, the stronger the covalent bond.

2.8   The shapes of simple molecules and ions 2.2.2

You need to know   the shapes of, and bonding angles in, molecules and ions with up to six electron pairs (including lone pairs) surrounding the central atom as predicted by electron pair repulsion.

Electron pair repulsion is a modal used for explaining and predicting shapes of covalently bonded molecules. It works on the principle that electron pairs, you guessed it, repel. They arrange themselves around an atom as wide apart as possible. They do this in 3D, which may sound obvious, but so far in chemistry we have worked only with 2D models. To draw 3D diagrams we need to understand the following standards,

- A——B is used for a bond in the same plane as the paper

- A◀B is used for a bond coming out of the paper

- A ⋯⁣ıⅡⅠB is for bonds going into the plane of the paper

Bonded pair/lone pair repulsion is stronger than bonded pair/bonded pair. This is because the lone pair of electrons occupying more space than the bonded pair, overall resulting in a slightly higher repulsion from the lone pair. The bonding angle is, therefore, reduced by around 2.5°for every lone pair.

Common, and basic examples are molecules such as, CH_4 which has a bonding angle of 109.5°and no loan pairs and forms a tetrahedral structure; NH_3 which has a bonding angle of 107°with one lone pair and this is pyramidal; finally H_2O which is non-linear and with its two lone pairs has a bonding angle of 104.5°.

The last shapes to be familiar with are trigonal planar which have a bonding angle of 120°, linear which are 180°and octahedral which are 90°. (I may add diagrams if I get time but page 71-72 of the textbook has good ones.)

2.9 Electronegativity and bond polarity 2.2.2

The Pauling scale is a scale used to measure the electronegativity of an atom. As we go right, across the periodic table, the electronegative increases along side a decrease in atomic radius. As we move up the table we see an decrease in the number of shells, hence a decrease in atomic radius, so we see then an increase in electronegativity. So the nearer F in the table, the higher the electronegitivity.

Electronegitivity simply refers to the amount of attraction a atom in a covalent bond has over the shared pair of electrons in a covalent bond.

Polar bonds are covalent bonds between two elements with different electronegitivities. $H^{\delta+} - Cl^{\delta-}$ is an example of a polar bond, and by extension a polar molecule. H has a lower electronegativity than chlorine causing the chlorine in the covalent bond to become slightly negative. This type of bonding is called a permanent dipole.

Covalent, Polar covalent and ionic   are defined here by the difference in electronegitivity of the bonding atoms. Where the difference is zero we call the bond covalent. Where it is less than 1.8 we call it polar covalent and where it is greater than 1.8 we call it ionic.

Larger molecules   are interesting in the sense that a we need to look at structure to see if the overall molecule is polar or non-polar. Take H_2O, this has a non-liner structure. Both the $H^{\delta+}\!-\!O^{\delta-}$ bonds are polar and given its non-liner structure, these polar bonds don't cancel out. This makes H_2O a polar molecule because it has an overall dipole.

However, take CO_2, a similar covalent molecule with two $C^{\delta+}\!=\!O^{\delta-}$ polar bonds. But this is where it changes. The structure is liner. This means that the two bonds cancel out $O^{\delta-}\!=\!C^{\delta+}\!=\!O^{\delta-}$. Meaning that the overall molecule, in the case of CO_2, is non-polar.

2.10   Intermolecular Forces 2.2.2

An important distinction from ionic or covalent bonding is that these are forces between separate molecules.

Permanent dipole - dipole interactions   are caused by polar molecules attracting each other and forming a permanent electrostatic interaction. This is very similar to giant ionic lattices but occurs with polar covalent molecules such as water. The distinction is that it is between separate molecules.

Generally permanent dipole interactions are conducive to a higher boiling point, given the extra energy required to break the interaction.

Hydrogen bonding   is "intermolecular bonding between molecules containing N, O or F and the H atom of –NH, –OH or HF". It is a special type of permanent dipole-dipole interaction.

Hydrogen bonding has a significant influence on the properties of many molecules. Water, for example, is affected by hydrogen bonding. Hydrogen bonding allows for the formation of a more open lattice structure by holding the molecules apart. The result is that ice is less dense than liquid water.

London Forces   are temporary dipole-dipole interactions. Electrons move, and as such may cause a molecule to be temporarily polar. This temporary polarity may allow the formation of an instantaneous dipole. This, on a micro scale, isn't a long lasting, however when we look on a macro scale with a massive number of molecules this has a large affect. This interaction occurs in every molecule.

London forces strength is dependant on the number of electrons. Elements with large number of electrons have stronger London forces due to the greater

probability of an interaction. So as we move down the periodic table we would expect a higher boiling point (where london forces are the primary interaction).

Simple molecular lattices   are formed when a simple molecular substance[2] are in there solid form. They are simply put "covalently bonded molecules attracted by intermolecular forces, e.g. I_2, ice". The molecules in simple covalent lattice are held together by repetitively *week* intermolecular forces, The atoms within the molecules are held together by very *strong* covalent bonds.

Solubility   of these different types of compounds follow this basic rule, in general: Polar compounds will be soluble in polar solvents and non-polar compounds will be soluble in non-polar solvents.

The reason for the polar compounds being soluble in polar solvents is that the polar solvent attracts the polar compound. This attraction, in a similar way to ionic compounds, acts to pull apart the permanent dipole-dipole bonds and causing the compound to dissolve.

The reason for the non-polar compounds dissolving in non-polar solvents is much the same. The intermolecular interactions are the same so the solvent is able to break down the simple covalent lattice.

Electrical conductivity   is nil for simple covalent structures. There are no mobile charged particles meaning that there will be no way for the substance to be conductive.

---

[2]A simple molecular substance is one with a defined number of atoms and with definite formula

Module 3

Periodic table and energy

The focus of this module is inorganic and physical chemistry, the applications of energy use to everyday life and industrial processes, and current environmental concerns associated with sustainability.

3.1 The Periodic table 3.1.1

Simply put   the periodic table lists the known elements in order of atomic number[1] and also grouped by periods, or rows, which show the trends in physical and chemical properties.

Groups, or columns, generally contain chemicals of similar properties. This is because they all have the same amount of electrons missing in the outer shell[2].

First ionisation energy   is the amount of energy required to remove one electron from each atom in one mole of gaseous substance. There are several things which affect first ionisation energy which I will now go into. The first ionisation energy generally increases as we go across the period and decreases as we go down the group in general.

This is because as we move across the period the nuclear charge gets greater. This then affects the atomic radius, making it smaller. This means that the electrons on the outer shells are more attracted to the nucleus and so the first ionisation energy increase.

As we move down a group we

Take period 2. as we go across it and look at the first ionisation energies we see this Li<Be>B<C<N>O<F<Ne. The question is why is Be>B and N>O? This doesn't fit with our previous generalisations.

---

[1]A number derived from the number of protons
[2]Sort of true for first three periods

Oddities in the first ionisation energy   The first oddity we see is between Be>B. This is caused as a result of Be having a full s sub-shell and B having only one electron in the p sub-shell. Although a little odd at first glance this should become obvious. A full sub-shell is going to need more energy to remove an electron than a sub-shell with only one electron. So we see this s-p sub orbital trend in first ionisation energies

The second oddity is the N>O. This is caused by p-orbital reputation. As the p orbital fills to 4 it looks like this,
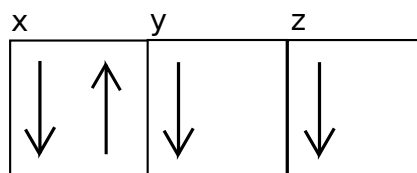
As we can see the P_x only has gained an electron of opposite spin. This causes repulsion which means that this new electron requires less energy to be removed than if we have P^3 like in Nitrogen. This is called p-orbital repulsion.

Successive ionisation energies   is what we see when we take several electrons away from an element. This can be used to predict the number of electrons in each shell. Between shells there is a large difference in ionisation energies.

Trends such as these give support to the Bohr model of the atom[3]. They support the idea that we have a variety of shells with sub-shells.

3.2   Periodic trend in structure 3.1.1

Metallic bonding   is the a "strong electrostatic attraction between cations (positive ions) and delocalised electrons". This bonding is between metals as forms giant metallic lattices. Metals are able to conduct electricity because of the sea of delocalised electrons created by the metallic bond. Metals are almost always solid at room temperature, except for mercury. This is because metallic bonding is very strong, but dependent on how many electrons the elements loose as well as well as other factors.

Giant covalent lattices   are, unlike simple molecular lattices, atoms not molecules bonded by covalent bonds. This can make for some incredibly strong elements. Carbon, boron and silicon are examples of atoms that can form giant covalent lattices. Carbon can form Diamond, graphite and graphene.

Other than graphite and graphene, giant covalent lattices will not conduct electricity. This is because the electrons are immobile. However graphite

---

[3]The Bohr model is the model you have been learning

has a free electron per carbon atom. These electrons join a sea of delocalised electrons and can move between the layers in the carbon. These mobile charge carriers are what allow graphite and graphene to be conductive.

Solubility Both metals and giant covalent lattices are, on the whole insoluble. In the case of metals, they may well react when in polar solvents not dissolve. In the case of giant covalent lattices, the bonding is far too strong to be broken by solvents.

Graphene is the latest wonder chemical. It consists of a single layer of graphite, composed of hexagonally linked carbon atoms. It has the same electrical conductivity of copper and is the thinnest, strongest element ever made. The reason for its electrical conductivity is that it has, like graphite, delocalised electrons. Theses act as mobile charge carriers.

There is potential for this to be used in micro-computing to replace silicone, this could server to further decrease the size and cost of computer processors.

Melting points for giant metallic/covalent structures are very heigh. This means the following (for periods 2 and 3):

- As we move from groups 1 to 14 we see a rise in melting temperatures as these elements form *giant structures*.

- A sharp drop is seen at group 14 to 15. This is because group 15-18 elements don't form giant structures.

- Group 15 to 18 are comparatively low. This is because are *simple molecular structures*.

3.3 Group 2 3.1.2

s sub-shell Is filled in all the group two elements. This means that they contain two more electrons than the Nobel gas before it. In redox reactions these substances loose two electrons and from 2+ ions.

The next part is just revisiting redox and so I will just summarise. You should know how group two elements from Mg$\rightarrow$Ba react with water, oxygen and week acids. Just know that group 2 elements are oxidised by +2.

Reactivity increases as we go down the group because the group two elements in a reaction loose electrons. So as we learnt before. As we move down the group the first (and in this case second) ionisation energies increase due

to greater shielding[4] and atomic radius (so overall less attraction to the outer s electrons.).

3.4   The halogens 3.1.3

Boiling trends   in halogens are caused because of there existence as diatomic molecules. The boiling point increases down the group because of the stronger London forces (caused by more electrons).

Redox again   is found here. Much the same as all the others but this time they are oxidised. This is because they need only gain one electron to have the electron configuration of a noble gas. They form anions.

Displacement reactions   occur when a significantly more reactive chemical is reacted with a compound containing a similar, but less reactive, compound. Using displacement reactions we can see that reactivity decreases down the group.

Halogen-halide displacement   The reactions are as follows,

- a chloride solution will not be displaced by bromine or iodine. This is because chlorine is the most reactive.

- a bromide solution will react when chlorine is added. It will turn orange as the Br^- ions are displaced and so from Br_2,

  $Cl_2(aq) + 2\,Br^-(aq) \longrightarrow 2\,Cl^-(aq) + Br_2(aq)$ However given that iodine is less reactive still there will be no reaction between I_2 and bromide.

- As the least reactive iodide solution will be displaced by both chlorine and bromine to form a brown solution,

  $Cl_2(aq) + 2\,I^-(aq) \longrightarrow 2\,Cl^-(aq) + I_2(aq)$

 $Br_2(aq) + 2\,I^-(aq) \longrightarrow 2\,Br^-(aq) + I_2(aq)$
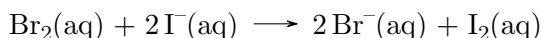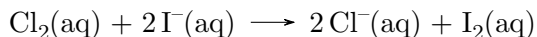
To tell apart the similar brown and orange we can add a non-polar solvent like cyclohexane to dissolve the halogen. When I_2 is dissolved we can see the cyclohexane layer go a deep violet.

The reason for decreasing reactivity   is that it is the opposite to group two. To gain an electron we need more attraction. As such more shielding and a grater atomic radius just cause less attraction to the electron and make it less reactive.

---

[4]Shielding is where electrons from other shells block, in a sense, the positive attraction on the outer electrons.

Disproportionation is what we call a reaction when the same element undergoes reduction and oxidation. This is illustrated by the following,

- The treatment of water with chlorine

$$\overset{0}{Cl}_2(aq) + H_2O(l) \longrightarrow H\overset{I}{Cl}O(aq) + H\overset{-I}{Cl}(aq)$$
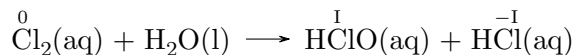
  As we can see, Chlorine has been both oxidised and reduced.

- The reaction of chlorine with cold, dilute aqueous sodium hydroxide,

$$\overset{0}{Cl}_2(aq) + 2\,NaOH(aq) \longrightarrow Na\overset{I}{Cl}O(aq) + Na\overset{-I}{Cl}(aq) + H_2O(l)$$
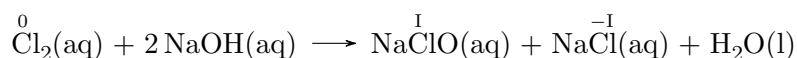
Water treatment using chlorine is extremely useful. This is because chlorine kills bacteria. However, there are some hazards in using chlorine. Toxic chlorine gas and the risk of forming carcinogenic chlorinated hydrocarbons (when reacting with plant matter).

The Halide tests are reactions used to test for halide ions in aqueous solution. This is done by adding aqueous silver ions (by using $AgNO_3$). The ionic equation is as follows (where X is any halide ion),

$$Ag^+(aq) + X^-(aq) \longrightarrow AgX(s)$$
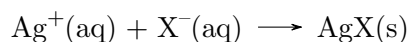
As we can see, this reaction creates a precipitate. Now we can derive the precise halide ion by looking at the colour of the precipitate. Chlorine will form a white precipitate, Bromine a cream and iodine yellow.

Adding dilute aqueous ammonia will dissolve the precipitate AgCl, and by adding concentrated aqueous ammonia we dissolve both AgCl and AgBr.

3.5 More tests 3.1.4

Three tests you need to know for this section. They need to be done in the following order,

1. Carbonate (CO_3^{2-}(aq)) test

2. Sulfate (SO_4^{2-}(aq)) test

3. halide (Cl^-(aq),Br^-(aq) and I^-(aq)) test

Carbonate ions are tested by adding a dilute acid. It is by the following ionic equations,

$$CO_3^{2-}(aq) + 2\,H^+(aq) \longrightarrow H_2O(l) + CO_2(g)$$
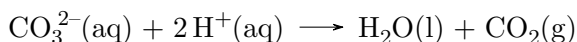
As you can see CO_2 is formed, which is gaseous. So if a $CO_3^-(aq)$ ion is present we will see effervescence when we add it. We will see why we need to do this first. (remember to use an acid which will not interfere in the other two tests like NHO_3.

Sulphate ions are tested for by adding $Ba^{2+}(aq)$. This is now by the following equations,

$$Ba^{2+}(aq) + SO_4^{2-} \longrightarrow BaSO_4(s)$$
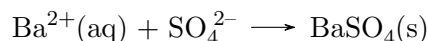
We see a white precipitate form ($BaSO_4(s)$). However this needs to be done after the carbonate test because Ba^{2+} ions will form $BaCO_3(s)$, which is also a white precipitate.

The halide tests are mentioned above.

Testing for ammonium ions is simple. Just react with warm aqueous NaOH,

$$OH^-(aq) + NH_4^+(aq) \longrightarrow NH_3(g) + H_2O(l)$$
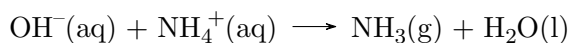
So by adding NaOH we will see the solution effervesce if the NH_4^+ ions.

3.6   Enthalpy 3.2.1

[For now I am skipping this section due to is easiness. Just apply basic logic and maths]

3.7   Rates of Reaction 3.2.2

Collision theory hasn't changed at all from GCSE. Sill we look at the microscopic consequences of pressure, concentration and temperature (kinetic energy) on individual molecules. Successful collisions are needed which is when the reactive atoms in a molecule collide.

Catalysts are substances that, when added to a chemical reaction, serve to increase the rate of reaction without reacting itself.

This effect is achieved by the catalyst decreasing the required activation energy, thus providing a faster pathway for the reaction to take place.

Homogeneous catalysts refers to a catalyst that is in the same state as the reactants. This works by forming intermediate products.

Heterogeneous catalysts are catalysts which differ in state from the reactants. These act by a series of absorption and desorption.

Catalysts have massive importance in industry. They are used to reduce the amount of energy (in heat and pressure) in industrial reactions. This then reduces the amount of fossil fuels needing to be burnt, thus reducing CO_2.

Measuring rates of reaction can be done in many ways. This can involve measuring gas or mass over time.

The Boltzmann distribution is a frequency distribution used to predict the energy of molecules. The area under the curve represents the number of molecules with a given energy. The curve changes when the temperature rises (skews negativity). E_a moves to the left when a catalyst is added.

3.8 Chemical equilibrium 3.2.3

A dynamic equilibrium exists in a closed system when the rate of the forward reaction is equal to the rate of the reverse reaction and the concentrations of reactants and products do not change.

le Chatelier's principle states that "When any system at equilibrium is subjected to change in concentration, temperature, volume, or pressure, then the system readjusts itself to (partially) counteract the effect of the applied change and a new equilibrium is established."

Remember that catalysts do not affect the position of equilibrium as they only affect the activation energy, and the reaction goes both ways so this cancels out.

Investigating equilibrium with concentration is done by the following,

$$2\,CrO_4^{2-}(aq) + 2\,H^+(aq) \rightleftharpoons Cr_2O_7^{2-}(aq) + H_2O(l)$$
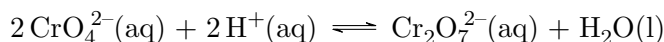
This reaction is sensitive to the acid concentration. Adding acid concentration will shift the point of equilibrium to the 'right'. We can see this because $CrO_4^{2-}(aq)$ solution is yellow and $Cr_2O_7^{2-}(aq)$ solution is yellow. So by raising the concentration of the acid we see the solution got from yellow to orange. Procedure is as follows:

1. Add a solution of yellow potassium chromate to a beaker

2. Add dilute sulfuric acid drop by drop until there is no further change in colour (orange).

3. Add aqueous sodium hydroxide until there is no further change in colour (yellow).

You have now witnessed equilibrium in action.

Investigating equilibrium with temperature is done by the following,

$$[Co(H_2O)_6]^{2+}(aq) + 4\,Cl^-(aq) \rightleftharpoons CoCl_4^{2-}(aq) + 6\,H_2O(l)$$
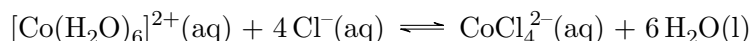
As temperature increases the reaction shifts right (in the endothermic direction) and vice-versa. This reaction can be done by the following steps,

1. Dissolve cobalt chloride in a boiling tube. Add a small quantity of hydrochloric acid. Then put the solution in ice to cool it until it turns pink (because $[Co(H_2O)_6]^{2+}(aq)$ solution is pink).

2. Set up a boiling water bath and transfer the boiling tube. Wait until it turns blue (because $CoCL_4^{2-}$ is blue).

3. Transfer back to ice water and observe the change back to pink.

And you have now witnessed a shift in equilibrium.

3.9 The equilibrium constant, K_c 3.2.3

Equilibrium constant is calculated by,

In the reaction $a\text{A} + b\text{B} \rightleftharpoons c\text{C} + d\text{D}$

$$K_c = \frac{[\text{C}]^c[\text{D}]^d}{[\text{A}]^a[\text{B}]^b} \tag{3.1}$$

This requires a little explaining, The A, B, C and D values are the *equilibrium* concentrations of the reactants (in mol dm^{-3}).

Where $K_c = 1$ it indicates that the reaction is halfway between reactants and products.

Where $K_c > 1$ it indicates that the position of equilibrium is shifted to the right (the products).

Where $K_c < 1$ it indicates that the position of equilibrium is shifted to the left (the reactants).

Module 4

Core organic chemistry

This module introduces organic chemistry and its important applications to everyday life, including current environmental concerns associated with sustainability.

4.1 The basics 4.1.1

IUPAC rules on the nomenclature of organic compounds is as follows,

Firstly let me explain the parts of the name. Stem, prefix and suffix. The stem refers to the number of carbon atoms in the longest chain (just remember Monkeys Eat Peanut Butter + Greek); the prefix is in reference to a side chain (or a functional group); the suffix is added to indicate functional groups.

We have three types of hydrocarbons, aliphatic, acyclic and aromatic. We will mostly focus on aliphatic hydrocarbons of which there are three homologous[1] series alkanes, alkenes and alkynes.

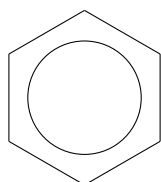**Aliphatic** hydrocarbons are one which are joined in chains e.g,

2-methylethane

---
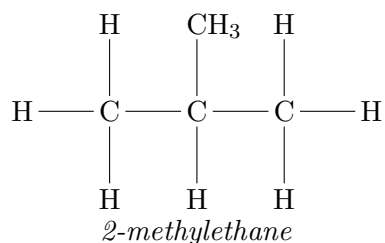
[1]A group of chemicals with the same functional group, differing by an addition of CH_2

25

Alicyclic   hydrocarbons join in cyclic shapes and look like this,
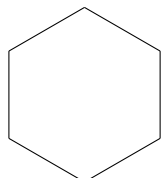
Cyclohexane

Aromatic   hydrocarbons have benzene rings which contain all or some of the carbon atoms,

Benzene

Functional groups (prefixes)   are as follows,

| Functional group	Prefix	Suffix	Displayed
carboxylic acids	none	-oic acid	
aldehydes	none	-al	
ketones	none	-one	
alchols	hydroxy-	-ol	
amines	amino-	-amine	
ethers	alkoxy-	-ether	
fluorine	fluoro-	none	
chlorine	chloro-	none	
bromine	bromo-	none	
iodine	iodo-	none	

I included a few more, I should imagine you only need the first 3 and the haloalkane ones (given that they are the ones in the textbook).

Displaying formula   There are three ways to display chemical formula (for the exam). These being the following,

General formula is the simplest algebraic formula of a member of a homologous series. For example, for an alkane C_nH_{2n+2}.

Structural formula is the minimal detail that shows the arrangement of atoms in a molecule. We write out each alkile group[2] and there surrounding atoms. E.g. for 2,4-pentandione we have $CH_3COCH_2COCH_3$.

Displayed formula is where the full molecule is drawn so in the case of 2,4-pentandione,
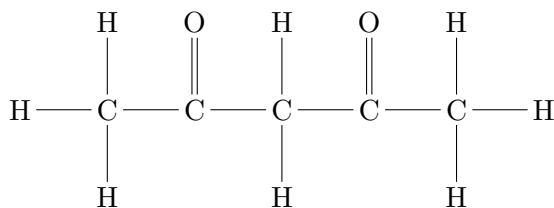
Skeletal formula is the simplified organic formula, shown by removing hydrogen atoms from alkyl chains, leaving just a carbon skeleton and associated functional groups. So in the case of 2,4-pentandione,
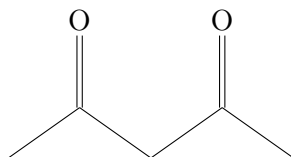
Definition   time (and summary, straight from the horse's mouth),

- homologous series (a series of organic compounds having the same functional group but with each successive member differing by CH_2)

- functional group (a group of atoms responsible for the characteristic reactions of a compound)

- alkyl group (of formula C_nH_{2n+1})

- aliphatic (a compound containing carbon and hydrogen joined together in straight chains, branched chains or non-aromatic rings)

- alicyclic (an aliphatic compound arranged in non-aromatic rings with or without side chains)

- aromatic (a compound containing a benzene ring)

- saturated (single carbon–carbon bonds only) and unsaturated (the presence of multiple carbon–carbon bonds, including C=C, C/C and aromatic rings)

---

[2]C atoms in the main chain

Structural isomers are compounds with the same molecular formula but different structural formulae. Take, for C_4H_{10}. Sound simple,

But now imagine a possible combination that could share the same molecular formula,
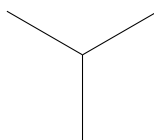
This is called a structural isomer. Both 2-methylpropane and butane are C_4H_{10}. This is where structural formula and skeletal diagrams come in handy.

4.2 Reaction Mechanisms 4.1.1

Homolytic fission is where a covalent bond breaks and the electrons are shared evenly with each bonding atom receiving one electron from the bonded pair, forming two radicals.

Heterolytic fission is where a covalent bond breaks and the electrons are not shared evenly with one bonding atom receiving both electrons from the bonded pair.

Radicals are a species with an unpaired electron. We use a dot to show this, e.g. $H_3C-CH_3 \longrightarrow H_3C\bullet + CH_3\bullet$. This being homolytic fission as each bonded atom receives one electron.

Curly arrows are used to describe the movement of an electron pair. They show either heterolytic fission or the formation of a covalent bond.

Reaction mechanism diagrams are used to show reaction mechanisms. They need to be sufficiently detailed, to show clearly the movements of an electron pair, with curly arrows and relevant dipoles.

4.3 Alkanes 4.1.2

Alkanes are saturated hydrocarbons containing single C–C and C–H bonds as σ-bonds (overlap of orbitals directly between the bonding atoms); free rotation of the σ-bond.

**A σ-bond** is the result of two overlapping orbital in. It is a single covalent bond.

The bond angle formed when a carbon atom has 4 σ-bonds is 109.5°.

Trends in boiling points are also obvious. The larger the molecule the more London forces there are at play. This means that the larger the molecule the more energy is needed to break the intermolecular forces and hence boiling the alkane. We also see the boiling point lower if the molecules branch. This is due to less surface area.

Reactivity of alkanes is low. This is because of the relative stability[3] and very low polarity of the σ-bonds.

The combustion of alkanes is seen everywhere. This is because fossil fuels like methane are alkanes. The longer the chain the more energy released per mole. The combustion reaction is as standard producing CO_2 and H_2O.

Alkanes and halogens can react in the presence of UV radiation,

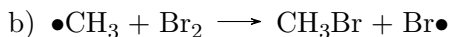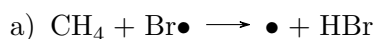$$CH_4(g) + Br_2(l) \xrightarrow{\text{UV}} CH_3Br(g) + HBr(g)$$
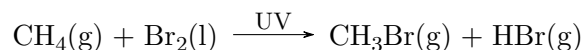
However you need to know the mechanism of this reaction. It is as follows:

1. First the bond in the bromine molecule is broken up by homolytic fission
   $Br{-}Br \xrightarrow{\text{UV}} Br\bullet + \bullet Br$
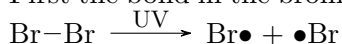
2. Next we have the propagation steps. This forms a chain reaction,

   a) $CH_4 + Br\bullet \longrightarrow \bullet + HBr$

   b) $\bullet CH_3 + Br_2 \longrightarrow CH_3Br + Br\bullet$

3. Finaly there is the termination, in which the two radicals collide forming a molicule with all the electron pairs. There are a number of ways this could happen.

   - $Br\bullet + \bullet Br \longrightarrow Br_2$
   - $\bullet CH_3 + \bullet CH_3 \longrightarrow C_2H_6$
   - $\bullet CH_3 + \bullet Br \longrightarrow CH_3Br$

---

[3]High bond enthalpy

4.4   Basics in Alkenes 4.1.3

Alkenes   are unsaturated hydrocarbons containing a C=C bond comprising a π-bond (sideways overlap of adjacent p-orbitals above and below the bonding C atoms) and a σ-bond (overlap of orbitals directly between the bonding atoms). The π bonds prevent the C=C bond from rotating freely. I will explain later.

The structure   is trigonal planar with the bonding angle around each C=C alkenes is 120°.
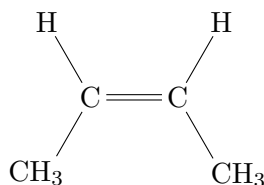
Stereoisomers   are compounds with the same structural formula but with a different arrangement in space. We look at E/Z isomerism. This is when we see stereoisomers are formed due to a restriction of rotation around the C=C group.

cis–trans isomerism   special case of E/Z isomerism in which two of the substituent groups attached to each carbon atom of the C=C group are the same.

Cahn–Ingold–Prelog (CIP) priority rules   are used to strictly define EZ isomers. It is based on 'priority' of the atoms bonded to the C=Cs. The 'priority' is down to the relative height of atomic number.

$$\begin{array}{ccc} CH_3 & & H \\ & C=C & \\ H & & CH_3 \end{array}$$
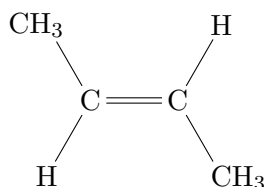
Will be an E isomer because C has a higher atomic number than H.

$$\begin{array}{ccc} H & & H \\ & C=C & \\ CH_3 & & CH_3 \end{array}$$

And be a Z isomer.